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Synthesis of Polycyclic Aromatic Hydrocarbons via Phenyl Addition – Dehydrocyclization: The Third Way

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Abstract: Polycyclic Aromatic Hydrocarbons (PAHs) represent the link between resonance-stabilized free radicals and carbonaceous nanoparticles generated in incomplete combustion processes and in circumstellar envelopes of carbon rich Asymptotic Giant Branch (AGB) stars. Although these PAHs resemble building blocks of complex carbonaceous nanostructures, their fundamental formation mechanisms have remained elusive. By exploring these reaction mechanisms of the phenyl radical with biphenyl/naphthalene theoretically and experimentally, we provide compelling evidence on a novel Phenyl-Addition/dehydroCyclization (PAC) pathway leading to prototype PAHs: triphenylene and fluoranthene. PAC operates efficiently at high temperatures leading through rapid molecular mass growth processes to complex aromatic structures, which are difficult to synthesize via traditional pathways such as Hydrogen-Abstraction/Acetylene-Addition. The elucidation of the fundamental reactions leading to PAHs is necessary to facilitate an understanding of the origin and evolution of the molecular universe and, in particular, of carbon in our Galaxy.

Introduction

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For decades, polycyclic aromatic hydrocarbons (PAHs) – organic molecules featuring laterally fused benzene rings^[1] - have been at the center of attention as prospective candidates to untangle the molecular carriers of the unidentified infrared (UIR) emissions^[2] and of the diffuse interstellar bands (DIBs).^[2] These surveys propose that PAHs may encompass up to 20% of the galactic carbon budget^[3] and act as a link between resonantly stabilized free radicals (RSFRs)^[4] and carbonaceous nanoparticles in interstellar and circumstellar environments.^[5] The detection of PAHs in carbonaceous chondrites such as Murchison along with ¹³C/¹²C isotopic analyses advocates an extraterrestrial origin of PAHs^[1, 6] with fundamental astrochemical models of PAH synthesis borrowed from the combustion community.^[7] The Hydrogen-Abstraction/Acetylene-Addition (HACA) mechanism has been suggested to be important in the formation of PAHs in outflows of carbon-rich asymptotic giant branch (AGB) stars^[8] and in the combustion of fossil fuel.^[9] A repetitive sequence of an abstraction of a hydrogen atom from the aromatic hydrocarbon followed by an addition of acetylene (C₂H₂) prior to cyclization and aromatization lead to PAHs carrying up to four fused benzene rings - naphthalene (C₁₀H₈),^[7a] phenanthrene (C₁₄H₁₀),^[7c, 10] and pyrene (C₁₆H₁₀)^[11] – can be synthesized at high temperatures involving HACA. Recently, the the Hydrogen-Abstraction/Vinylacetylene-Addition (HAVA) mechanism has been invoked since naphthalene (C₁₀H₈),^[12] phenanthrene (C₁₄H₁₀), and anthracene (C₁₄H₁₀)^[13] were shown to be synthesized via barrier-less collisions of phenyl (C₆H₅·) and naphthyl (C₁₀H₇·) radicals with vinylacetylene (C₄H₄) via ring annulation at temperatures as low as 10 K.

Despite their potential in synthesizing PAHs in extreme environments, both the HAVA and HACA mechanisms have come under scrutiny, since flame data and recent models infer that a stepwise addition of acetylene is too slow to reproduce the quantified mass fractions of PAHs in combustion flames and in circumstellar environments.^[14] Koshi et al.^[15] along with Li et al.^[16] postulated that an overlooked Phenyl-Addition/dehydroCyclization (PAC) mechanism may result in a rapid synthesis of PAHs. This hypothetical PAC route involves an addition of phenyl to an aromatic hydrocarbon. This is followed by hydrogen loss and successive dehydrogenation succeeded by cyclization along with another hydrogen atom loss accompanied by aromatization (Fig. 1). However, the validity of PAC has remained uncharted, since not a single experimental study could substantiate to what extent PAHs can form since all mechanisms – HACA, HAVA, and PAC – operate simultaneously in combustion environments. This complexity requires a systematic elucidation of the fundamental elementary reactions^[17] involved in the PAC route.

Here, we reveal the facile gas phase synthesis of two prototype PAHs – fluoranthene (C₁₆H₁₀) and triphenylene (C₁₈H₁₂) – via

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Phenyl-Addition/ dehydroCyclization (PAC) in high temperature environments (Fig. 1). This is achieved by first disentangling the previously elusive chemistry of the elementary reactions of phenyl ($C_6H_5^\bullet$) with biphenyl ($C_{12}H_{10}$) and naphthalene ($C_{10}H_8$) forming triphenylene ($C_{18}H_{12}$) and fluoranthene ($C_{16}H_{10}$), respectively. Then, we trace the reactivity of a prototype radical intermediate in PAC – 2-(1-naphthyl)phenyl ($C_{16}H_{11}^\bullet$) – and provide critical evidence on the role of key hydrocarbon radicals. These findings suggest PAC as a *third way* – besides HACA and HAVA – to efficiently synthesize PAHs serving as building blocks of two- and three-dimensional aromatic structures in combustion flames and in circumstellar envelopes. Briefly, a high temperature

chemical reactor was used to form fluoranthene ($C_{16}H_{10}$) and triphenylene ($C_{18}H_{12}$) via the reactions of the phenyl radical with naphthalene ($C_{10}H_8$) and biphenyl ($C_{12}H_{10}$), respectively; second, ring closure of the 2-(1-naphthyl) phenyl radical ($C_{16}H_{11}^\bullet$) followed by hydrogen loss and aromatization to fluoranthene ($C_{16}H_{10}$) highlights the key role of aromatic radical intermediates in the PAC mechanism. All products were detected isomer-specifically through fragment-free photoionization in a molecular beam via tunable vacuum ultraviolet light in tandem with the identification of the ionized molecules in a reflectron time-of-flight mass spectrometer (SI).

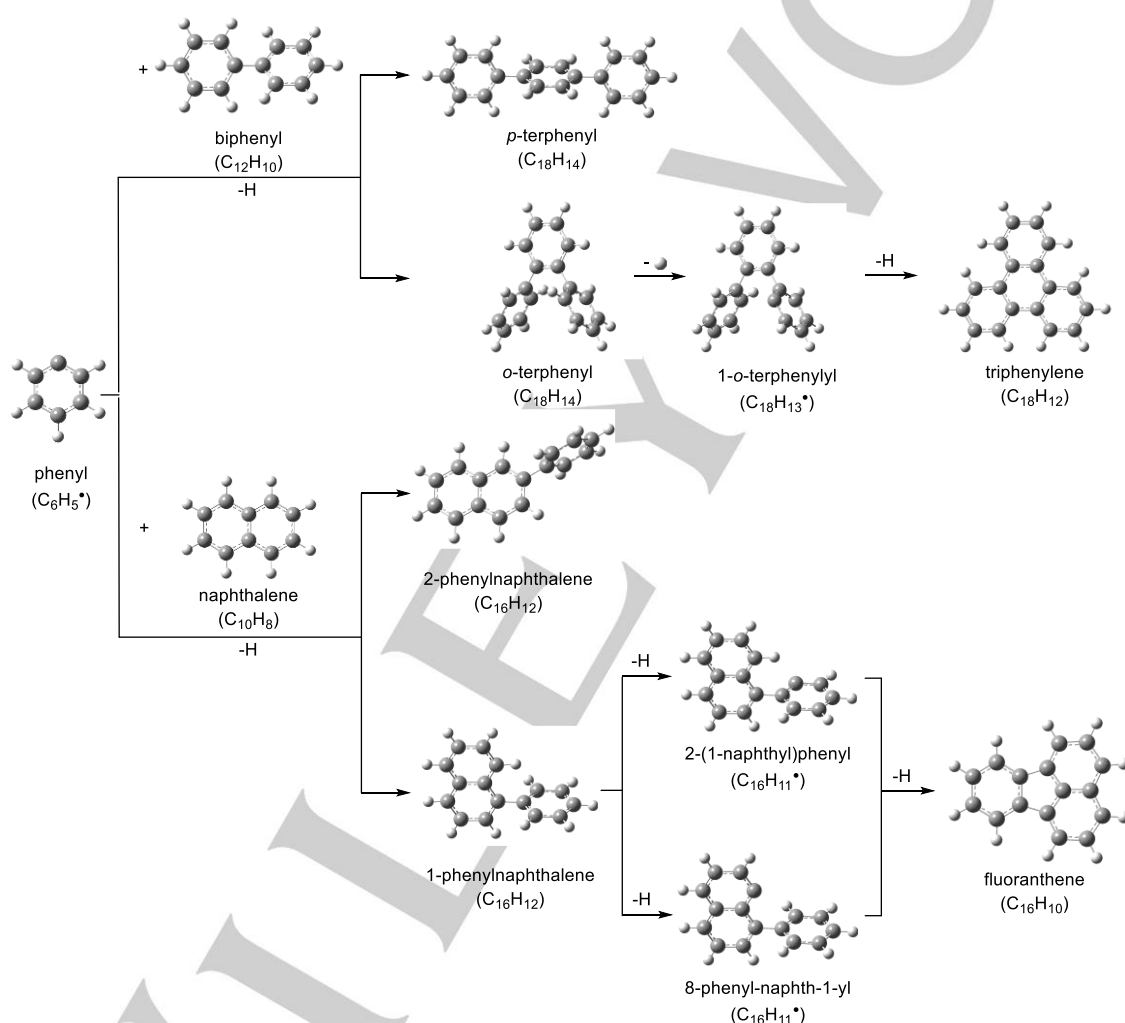


Figure 1. Postulated reactions leading to PAH formation via the Phenyl Addition/dehydro-Cyclization (PAC) mechanism. Carbon and hydrogen atoms are color coded gray and white, respectively.

Results and Discussion

Mass Spectra

Representative mass spectra recorded at a photoionization energy of 9.50 eV for the reactions of biphenyl and naphthalene

with the phenyl radical are displayed in Fig. 2. A comparison of these data with reference spectra obtained for biphenyl and naphthalene seeded in non-reactive helium gas provides evidence on the synthesis of molecules with the molecular formula $C_{18}H_{12}$ (228 amu) and $C_{18}H_{14}$ (230 amu) (Fig. 2a) as well as of $C_{16}H_{10}$ (202 amu) and $C_{16}H_{12}$ (204 amu) (Fig. 2c); these species are absent in the control experiments (Figs. 2b and 2d).

The following analysis allows us to gauge the reactivity of the 2-(1-naphthyl)phenyl radical intermediate ($C_{16}H_{11}$) (Figs. 2e,f). At 600K, the 1-(2-bromophenyl)naphthalene precursor molecule is assigned through the molecular ion peaks at $m/z = 282$ ($C_{16}H_{11}^{79}Br$), 283 ($^{13}CC_{15}H_{11}^{79}Br$), 284 ($C_{16}H_{11}^{81}Br$), and 285 ($^{13}CC_{15}H_{11}^{81}Br$) (Fig. 2f). When the temperature is increased to 1300K, new ion counts arise at $m/z = 202$ ($C_{16}H_{10}^+$), 203 ($C_{16}H_{11}^+ / ^{13}CC_{15}H_{10}^+$), and 204 ($C_{16}H_{12}^+$) (Fig. 2e). To further

identify the nature of the *isomers* formed in these systems, photoionization efficiency (PIE) curves, which record the intensities of an ion at a well-defined mass-to-charge ratio versus the photon energy, were collected between 7.5 to 10.0 eV. The experimentally recorded PIE curves are fit with a linear combination of known PIE calibration curves of distinct structural isomers to identify which molecule(s) is(are) synthesized.

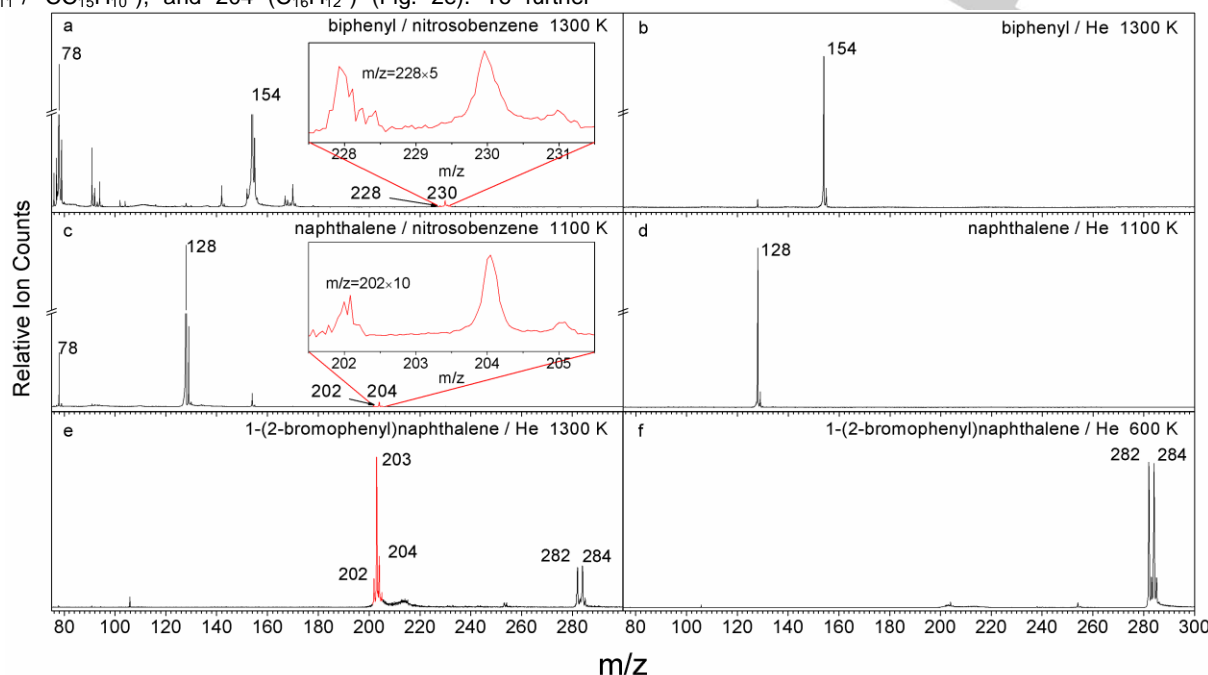
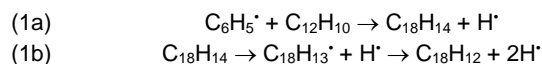


Figure 2. Comparison of photoionization mass spectra recorded at a photoionization energy of 9.50 eV. (a) biphenyl ($C_{12}H_{10}$)-nitrosobenzene (C_6H_5NO); the insert highlights the ion signals at $m/z = 228$; (b) biphenyl ($C_{12}H_{10}$)-helium (He); (c) naphthalene ($C_{10}H_8$)-nitrosobenzene (C_6H_5NO); the insert highlights the ion signals at $m/z = 202$; (d) naphthalene ($C_{10}H_8$)-helium; pyrolysis of 1-(2-bromophenyl) naphthalene at 1300K (e) and 600K (f). Mass peaks of the newly formed species of interest are highlighted in red. The inserts magnify sections of the mass spectra.

Photoionization Efficiency (PIE) Curves

In the biphenyl – phenyl system, accounting for the molecular weight of the reactants ($C_{12}H_{10}$, 154 amu; $C_6H_5^*$, 77 amu) and the products ($C_{18}H_{14}$, 230 amu; H, 1 amu), molecules with the formula $C_{18}H_{14}$ can be linked to reaction products of the elementary reaction of biphenyl with the phenyl radical (Figs. 2a,b) with ion count at $m/z = 231$ connected to ^{13}C -substituted counterpart of $m/z = 230$ ($^{13}CC_{17}H_{14}$) (reaction (1a)). Ion counts at $m/z = 230$ and 231 are absent in the control experiment suggesting that signals at these mass-to-charge ratios originate from *reaction* between the phenyl radical and biphenyl. Ion counts at $m/z = 77$ ($C_6H_5^+$), 78 ($C_6H_6^+ / C_5^{13}CH_5^+$), and 79 ($C_5^{13}CH_6^+$) are also observable; they are attributed to phenyl ($C_6H_5^+$), benzene (C_6H_6), and ^{13}C -benzene ($C_5^{13}CH_6$). Signal is also detectable at $m/z = 228$, which can be associated with two subsequent hydrogen atom losses and dehydrogenation from $C_{18}H_{14}$ via $C_{18}H_{13}^+$ to $C_{18}H_{12}^+$ (reaction (1b)). To summarize, the analysis of the mass spectra alone reveals that the reaction of the biphenyl ($C_{12}H_{10}$) with phenyl ($C_6H_5^*$) synthesizes hydrocarbon molecule(s) with the molecular formulae $C_{18}H_{12}$ and $C_{18}H_{14}$. To identify the structural isomers formed, the PIE curves recorded at $m/z = 228$, 230 and 231 are analyzed (Figs.

3a-c). For $m/z = 230$ and 231, the experimental PIE curves depict onsets of the ion counts at 7.85 ± 0.05 eV, which agree very well with the adiabatic ionization energy of *p*-terphenyl of 7.80 ± 0.03 eV.^[18] After scaling, both PIE graphs at $m/z = 230$ and 231 are identical and can be replicated with the PIE curve of the *p*-terphenyl isomer (SI) (Figs. 3b and 3c) amplifying that signal at $m/z = 231$ originates from ^{13}C -labeled *p*-terphenyl ($^{13}CC_{17}H_{14}$). Most important, after scaling, the PIE curve at $m/z = 228$ does not overlap with the PIE curve at $m/z = 230$ suggesting that signal at $m/z = 228$ does not originate from fragments of $m/z = 230$. Here, the PIE curve at $m/z = 228$ can be reproduced with a PIE curve of triphenylene ($C_{18}H_{12}$) (SI) (Fig. 3a). The experimentally determined onset of ion counts at $m/z = 228$ at 7.85 ± 0.05 eV corresponds to the adiabatic ionization energy of triphenylene of 7.89 ± 0.04 eV.^[19] Consequently, our investigations reveal that in the phenyl – biphenyl system, molecular mass growth processes account for the formation of *p*-terphenyl ($C_{18}H_{14}$) and of triphenylene ($C_{18}H_{12}$) formed via reactions (1a) and (1b), respectively.



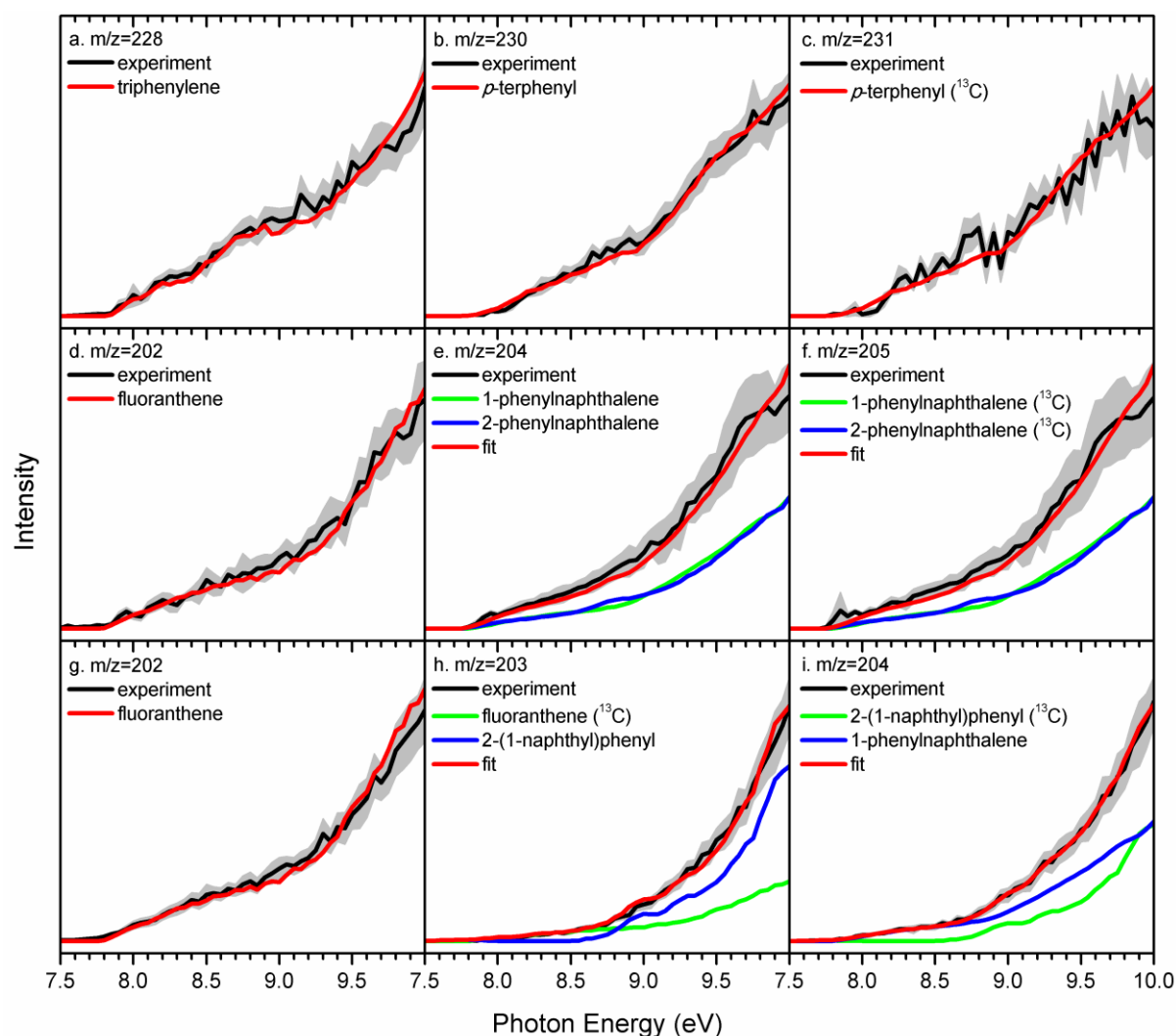
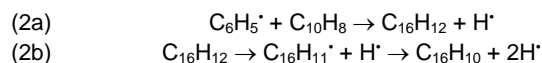


Figure 3. Photoionization efficiency (PIE) curves: (a)-(c): phenyl ($C_6H_5^+$) - biphenyl ($C_{12}H_{10}$); (d)-(f): phenyl ($C_6H_5^+$) - naphthalene ($C_{10}H_8$); (g)-(i): 1-(2-bromophenyl)naphthalene (1300K). Black: experimental PIE curves; blue/green/red: reference PIE curves; the red line resembles the overall fit.

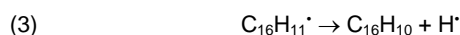
In the naphthalene – phenyl system, considering the molecular weight of the reactants ($C_{10}H_8$, 128 amu; $C_6H_5^+$, 77 amu) and the products ($C_{16}H_{12}$, 204 amu; H, 1 amu), molecules with the formula $C_{16}H_{12}$ are identified (Figs. 2c,d) with ion count at $m/z = 205$ correlated with the ^{13}C -substituted counterpart of $m/z = 204$ ($^{13}CC_{15}H_{12}$) (reaction (2a)). Since the ion counts at $m/z = 204$ and 205 cannot be detected in the control experiment, signals at both mass-to-charge ratios are linked to the reaction between the phenyl radical and naphthalene. Signal can be monitored at $m/z = 202$ as well. This is linked to two successive atomic hydrogen atom losses and dehydrogenation from $C_{16}H_{12}$ yielding ultimately $C_{16}H_{10}$ (reaction (2b)). Ion counts at $m/z = 77$ ($C_6H_5^+$), 78 ($C_6H_6^+/C_5^{13}CH_5^+$), 79 ($C_5^{13}CH_6^+$), 128 ($C_{10}H_8^+$), and 129 ($^{13}CC_9H_8^+$) can also be detected. The corresponding neutrals are phenyl (C_6H_5), benzene (C_6H_6), ^{13}C -benzene ($^{13}CC_5H_6$), naphthalene ($C_{10}H_8$), and ^{13}C - naphthalene ($^{13}CC_9H_8$). Thus, the mass spectra reveal that the reaction of naphthalene ($C_{10}H_8$) with phenyl (C_6H_5) synthesizes hydrocarbon molecules with the molecular formulae $C_{16}H_{12}$ and $C_{16}H_{10}$. To assign the isomers, the

PIE curves at $m/z = 202$, 204 and 205 are examined (Figs. 3d-f). At $m/z = 204$ and 205, both PIE graphs are superimposable after scaling and can be fit with a linear combination of the reference PIE graphs of 1- and 2-phenylnaphthalene (SI). Hence signal at $m/z = 205$ originates from $^{13}CC_{15}H_{12}$. The PIE calibration curves for 1- and 2-phenylnaphthalene isomers are nearly superimposable, and hence it is not feasible to determine accurate branching ratios of these isomers in the phenyl-naphthalene system. On the other hand, the PIE curves at $m/z = 202$ and 204 are distinct; data at $m/z = 202$ can be replicated with the PIE graph of fluoranthene ($C_{16}H_{10}$) (SI). The experimental onset of the ion counts at $m/z = 202$ at 7.85 ± 0.05 eV correlates nicely with the adiabatic ionization energy of fluoranthene of 7.90 ± 0.10 eV.^[20] Altogether, the experiments propose that in the phenyl – naphthalene system, 1- and/or 2-phenylnaphthalene ($C_{16}H_{12}$) along with fluoranthene ($C_{16}H_{10}$) are formed.



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Considering the 1-(2-bromophenyl)naphthalene system, signal at $m/z = 282$ ($C_{16}H_{11}^{79}Br$), 283 ($^{13}CC_{15}H_{11}^{79}Br$), 284 ($C_{16}H_{11}^{81}Br$), and 285 ($^{13}CC_{15}H_{11}^{81}Br$) is associated with the precursor molecules and their ^{13}C substituted counterparts. A detailed analysis of the PIE graphs in the 1300K experiment (Figs. 3g-i) reveals that ion counts at $m/z = 202$ are associated with fluoranthene ($C_{16}H_{10}$); the reference curves match the experimental data exceptionally well and reveal an onset of 7.80 ± 0.05 eV, which correlates nicely with the adiabatic ionization energy of fluoranthene of 7.90 ± 0.10 eV.^[20] The PIE graph at $m/z = 203$ ($C_{16}H_{11}^+ / ^{13}CC_{15}H_{10}^+$) can be replicated by a linear combination of the reference curves of ^{13}C -fluoranthene and the 2-(1-naphthyl)phenyl radical. Finally, the signal at $m/z = 204$ can be explained by 1-phenylnaphthalene formed, e.g., by hydrogen abstraction of the 2-(1-naphthyl)phenyl radical. In summary, our investigations reveal that the 2-(1-naphthyl)phenyl radical – a key intermediate in the PAC mechanism – undergoes isomerization via ring closure followed by atomic hydrogen loss yielding eventually fluoranthene ($C_{16}H_{10}$) (reaction (3), Fig. 1).



Reaction Mechanisms

Formation of Triphenylene

The present study reveals that two prototype PAHs carrying three and four benzene rings – triphenylene ($C_{18}H_{12}$) and fluoranthene ($C_{16}H_{10}$) – are synthesized within the phenyl–naphthalene and phenyl–biphenyl systems, respectively, in the gas phase. To elucidate the underlying reaction mechanisms, we combined

these findings with electronic structure calculations. Considering the reaction of the phenyl radical with biphenyl (reaction (1a)), the phenyl radical can add to the ortho (*o*-), meta (*m*-), and/or para (*p*-) position of the phenyl moiety of the biphenyl molecule through barrier up to 27 kJ mol^{-1} (Figs. 4a/4b). The resulting doublet radical intermediates **i1** to **i3** undergo hydrogen atom loss forming *o*-, *m*-, and *p*-terphenyl. Secondary reactions of atomic hydrogen and/or phenyl radicals with *o*-terphenyl lead via hydrogen abstraction to the 1-*o*-terphenyl (**i4**) radical, which can undergo facile cyclization to the doublet intermediate radical **i5**. Accompanied by aromatization, the latter undergoes unimolecular decomposition via atomic hydrogen loss forming triphenylene in overall exoergic reactions. Considering the heights of the barriers along with the overall reaction energies, the reaction of phenyl with *o*-terphenyl is favorable both kinetically and thermodynamically. These computations assist in rationalizing our experimental observations of the formation of *p*-terphenyl ($C_{18}H_{14}$) and triphenylene ($C_{18}H_{12}$). The initial replacement of a hydrogen atom by a phenyl group in the biphenyl reactant represents a prototype of an aromatic radical substitution reaction (S_R); this reaction favors the addition of the radical reactant to the *o*- and *p*-position of the phenyl moiety^[21] followed by atomic hydrogen loss leading to *o*- and *p*-terphenyl, but not to *m*-terphenyl. The *p*-terphenyl was observed experimentally; the absence of *o*-terphenyl, but the identification of triphenylene suggests an efficient conversion via dehydrogenation and cyclization of *o*-terphenyl to triphenylene (Fig. 1) thus demonstrating the unique capability of PAC to synthesize triphenylene.

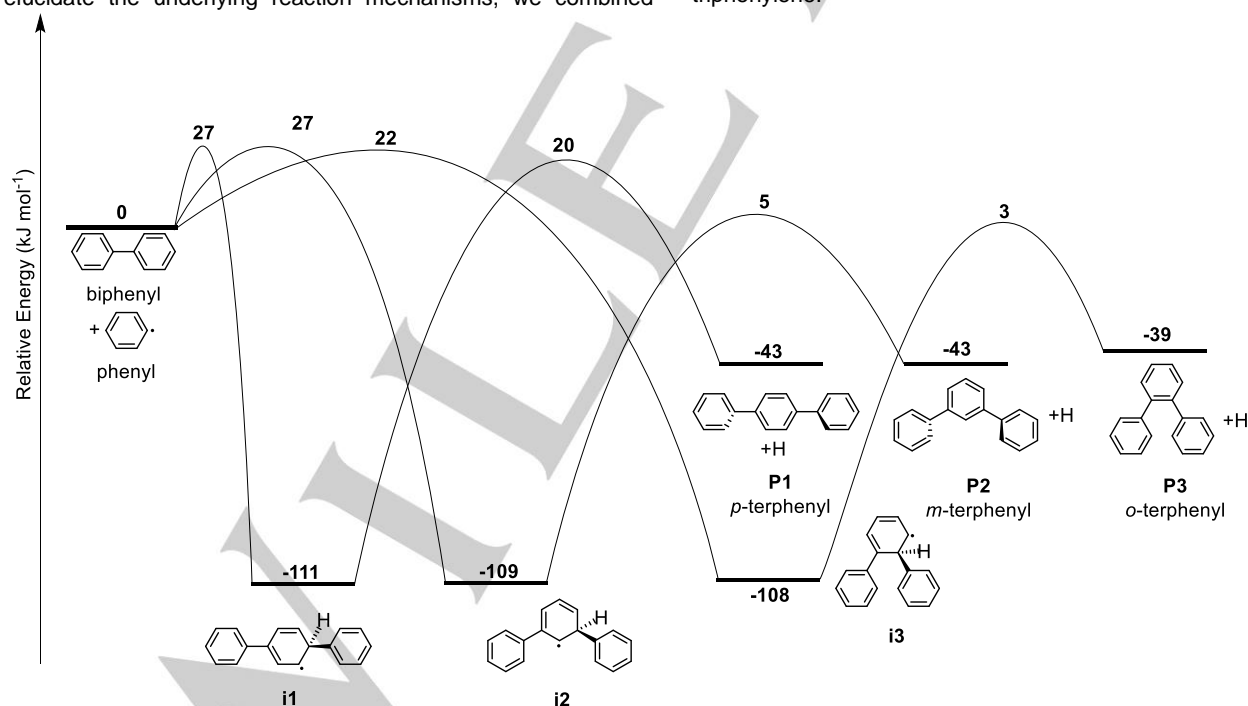


Figure 4a. Potential energy surface (PES) for the reaction of phenyl ($C_6H_5^{\cdot}$) with biphenyl ($C_{12}H_{10}$).

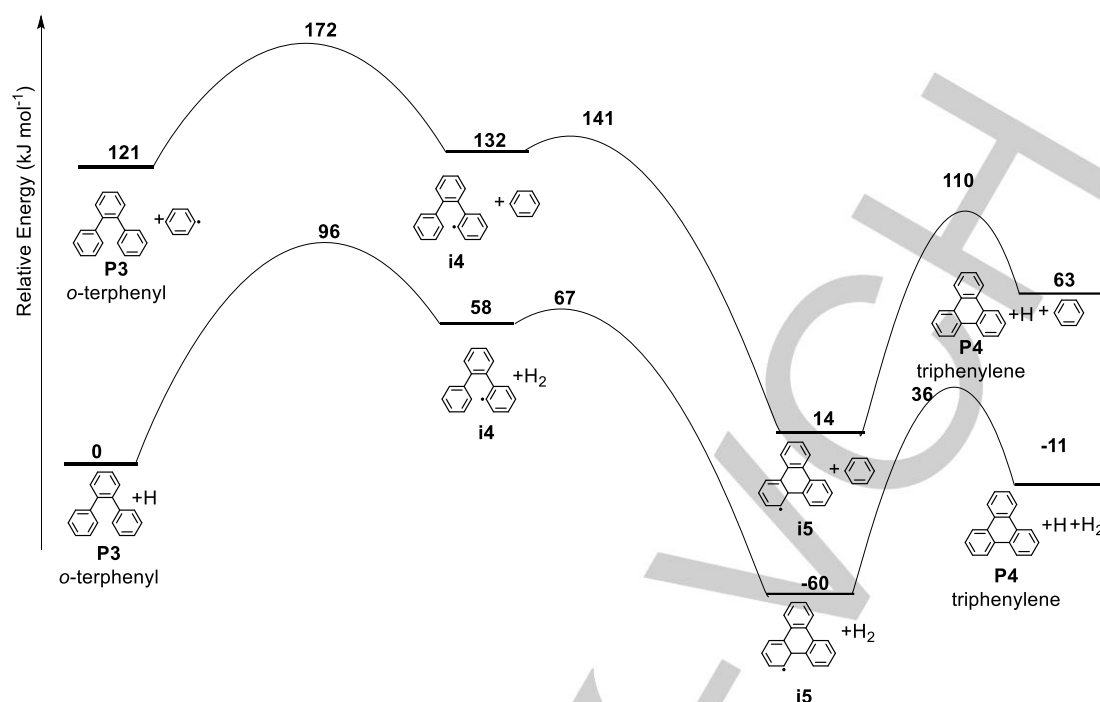


Figure 4b. Potential energy surface (PES) for the formation of triphenylene ($C_{18}H_{12}$) via hydrogen atom abstraction, cyclization, and hydrogen atom elimination.

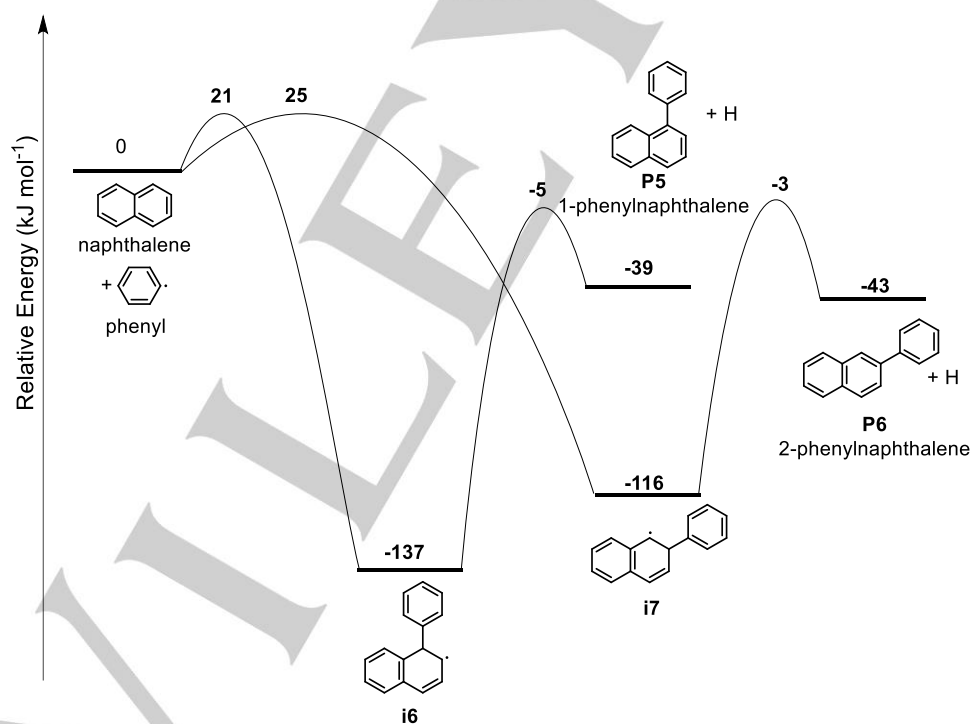


Figure 5a. Potential energy surface (PES) for the reaction of phenyl ($C_6H_5\cdot$) with naphthalene ($C_{10}H_8$).

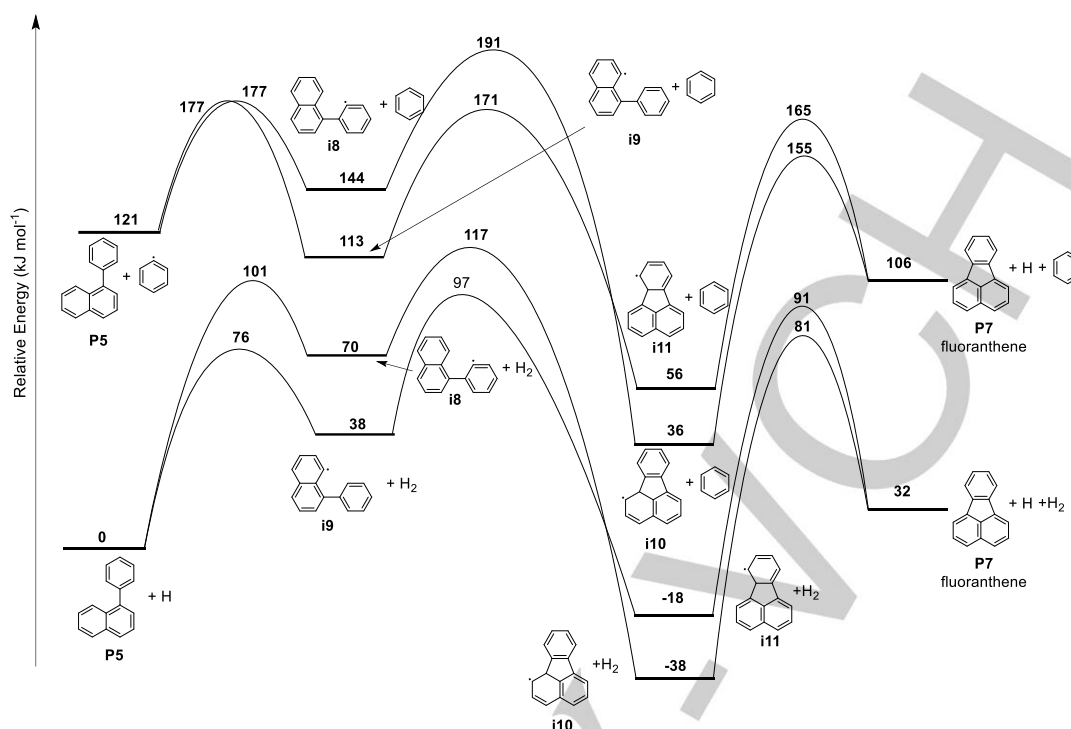


Figure 5b. Potential energy surface (PES) for the formation of fluoranthene ($C_{16}H_{10}$) via hydrogen atom abstraction, cyclization, and hydrogen atom elimination.

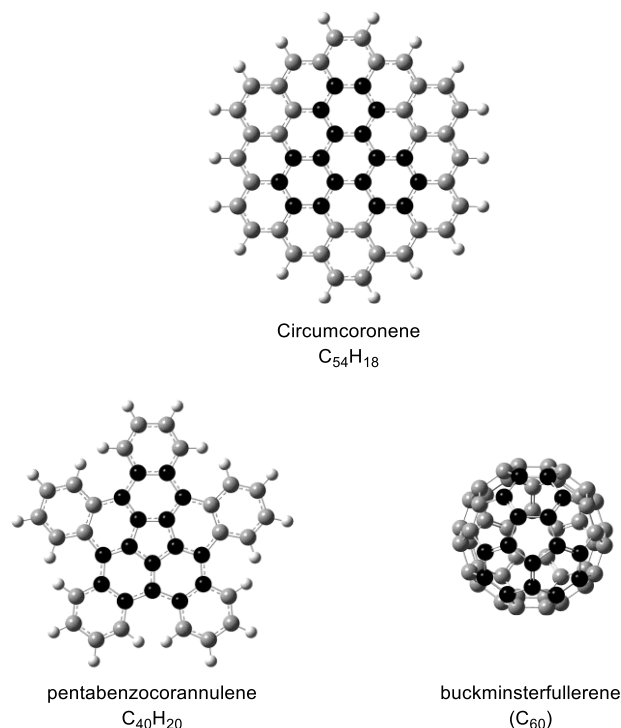
Formation of Fluoranthene

In the phenyl – naphthalene system (Fig. 5a), the phenyl radical adds to the C1 or C2 carbon atom of naphthalene yielding **i6** and **i7** doublet radical intermediates. These emit atomic hydrogen yielding 1-/2-phenylnaphthalene, respectively, in overall exoergic reactions. Secondary reaction of atomic hydrogen and/or phenyl radicals can abstract atomic hydrogen from 1-phenylnaphthalene. The hydrogen abstractions at the ortho positions of the phenyl and at the C8 carbon atom of the naphthalene moieties are critical to highlight. These abstractions lead to 2-(1-naphthyl)phenyl (**i8**) and 8-phenyl-naphth-1-yl (**i9**). Both the 2-(1-naphthyl)phenyl and 8-phenyl-naphth-1-yl radicals undergo cyclization to 1- and 7-H-fluoranthenyl **i10** and **i11**, respectively. Unimolecular decomposition of these intermediates via atomic hydrogen loss accompanied by aromatization forms fluoranthene (Fig. 5b). These predictions correlate well with our experimental findings and rationalize the identification of fluoranthene via PAC.

Conclusion

To conclude, our experimental data identified fluoranthene ($C_{16}H_{10}$) and triphenylene ($C_{18}H_{12}$) as key reaction products in the phenyl–biphenyl and phenyl–naphthalene systems with electronic structure calculations revealing the critical involvement of the previously elusive PAC mechanism. Since the initial addition of the phenyl radical to benzene and naphthalene along with the hydrogen abstraction from *o*-terphenyl and 1-phenylnaphthalene involve barriers of at least 21 kJ mol^{-1} , high temperature conditions in combustion processes and circumstellar envelopes

of carbon stars, are essential to an efficient mass growth processes to PAHs via PAC. The 18π aromatic triphenylene ($C_{18}H_{12}$) – a benchmark of a fully benzenoid PAH – and fluoranthene ($C_{16}H_{10}$) – a prototype of a non-alternant PAH – represent key molecular building blocks in molecular mass growth processes of two- and three-dimensional PAHs. These pathways may be involved in the formation of 2D and 3D nanostructures with buckminsterfullerene (C_{60}) detected in hydrocarbon flames^[22] and toward the planetary nebula TC 1 (Scheme 1).^[23] Overall, our findings establish a rigorous framework promoting PAC as a *third* way to synthesize PAHs via efficient molecular mass growth processes. In particular, the incorporation of a five-membered ring in PAHs such as fluoranthene, which has a dipole moment of 0.34 Debye, could aid in the detection of an individual PAH in the gas phase interstellar medium via its rotational spectrum exploiting the Atacama Large Millimeter/ submillimeter Array (ALMA) thus transforming how we think about the origin and evolution of carbonaceous matter in the Universe.^[24]



Scheme 1. Fluoranthene (C₁₆H₁₀) and triphenylene (C₁₈H₁₂) as molecular building blocks in two- and three-dimensional PAHs and fullerenes: circumcoronene (C₅₄H₁₈), pentabenzocorannulene (C₄₀H₂₀), and buckminsterfullerene (C₆₀).

Method

Experimental: The experiments were carried out at the Chemical Dynamics Beamline (9.0.2) of the Advanced Light Source utilizing a resistively-heated silicon-carbide (SiC) chemical reactor interfaced to a molecular beam apparatus operated with a Wiley-McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS).^[7a, 7b, 11–13, 25] The chemical reactor mimics the high temperature conditions present in combustion flames and in circumstellar envelopes of carbon stars. Phenyl radicals (C₆H₅•) were prepared *in situ* via pyrolysis of the nitrosobenzene precursor (C₆H₅NO; Sigma-Aldrich) with the biphenyl and naphthalene reactants provided by Sigma-Aldrich. The reactants were seeded in helium carrier gas (0.394 ± 0.005 atm). In the pyrolysis experiments, custom synthesized 1-(2-bromophenyl)naphthalene alone was seeded in the helium carrier gas at 0.394 ± 0.005 atm (Supplementary Information). The temperature of the SiC tube was monitored using a Type-C thermocouple and was maintained at 1300 ± 10 K (nitrosobenzene/biphenyl; 1-(2-bromophenyl)naphthalene) and 1100 ± 10 K (nitrosobenzene/naphthalene). The products formed in the reactor were expanded supersonically and passed through a 2 mm diameter skimmer located 10 mm downstream of the pyrolytic reactor and enter into the main chamber, which houses the Re-TOF-MS. The quasi-continuous tunable vacuum ultraviolet (VUV) light from the Advanced Light Source intercepted the neutral molecular beam perpendicularly in the extraction region of a Wiley–McLaren RE-TOF-MS. VUV single photon ionization is essentially a fragment-free ionization technique and hence is characterized as a *soft ionization* method compared to electron impact ionization, the latter leading to excessive fragmentation of the parent ion.^[26] The ions formed via photoionization are extracted and eventually detected by a microchannel plate detector. Photoionization efficiency (PIE) curves, which report ion counts as a function of photon energy with a step interval of 0.05 eV at a well-defined mass-to-charge ratio (*m/z*), were produced by

integrating the signal recorded at the specific *m/z* for the species of interest. Reference (blank) experiments were also conducted by expanding helium carrier gas into the resistively-heated SiC tube without seeding the reactants in nitrosobenzene. To identify the products of interest observed in this work, PIE calibration curves for 1-phenylnaphthalene, 2-phenylnaphthalene, fluoranthene, *o*-terphenyl, *m*-terphenyl, *p*-terphenyl, and triphenylene (Sigma Aldrich) were collected (Supplementary information). It is important to note that in blank experiments of nitrosobenzene seeded in helium carrier gas conducted at identical temperatures and pressures as the current experiments, naphthalene, triphenylene, or fluoranthene are not formed.^[7a]

Computational: The synthetic routes to triphenylene and fluoranthene are explored via electronic structure calculations. Along these routes, reactants, intermediates, products, and the transition states connecting these species are identified and characterized. Geometries and harmonic frequencies are optimized via density functional theory at the B3LYP^{[27]/cc-pVTZ level. The energies are refined by the coupled cluster^[28] CCSD(T)/cc-pVDZ with B3LYP/cc-pVTZ zero-point energy corrections. B3LYP/cc-pVTZ/CCSD(T)/cc-pVTZ level of calculation are expected to have an accuracy within 9 kJ mol^{−1}.^[29] The GAUSSIAN09 program^[30] is used in these electronic structure calculations.}

Acknowledgements

This work was supported by the US Department of Energy, Basic Energy Sciences DE-FG02-03ER15411 (experimental studies; synthesis of 1-(2-bromophenyl)naphthalene) to the University of Hawaii. BX, UA, and MA are supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, through the Gas Phase Chemical Physics program of the Chemical Sciences Division. The ALS is supported under the same contract. BJS, YLC, and AHHC thank the National Center for High-performance Computing in Taiwan for the computer resources.

Keywords: Phenyl-Addition/dehydroCyclization (PAC) • polycyclic aromatic hydrocarbons • gas-phase chemistry • mass spectrometry • interstellar medium

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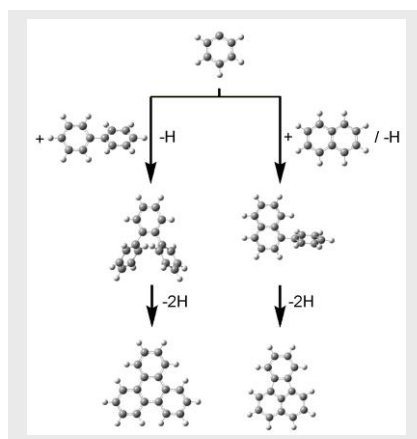
RESEARCH ARTICLE

Entry for the Table of Contents

Layout 1:

RESEARCH ARTICLE

The triphenylene and fluoranthene molecules – potential precursors to two- and three-dimensional graphitic nano sheets in the interstellar medium – can be formed through rapid molecular mass growth processes via the reactions of phenyl radical with biphenyl and naphthalene at high temperatures.



Long Zhao,^[a] Matthew Prendergast,^[a]
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Musahid Ahmed,^{[b]*} Bing-Jian Sun,^[c]
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Fischer^{[d,e,f]*}

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**Synthesis of Polycyclic Aromatic
Hydrocarbons via Phenyl Addition –
Dehydrocyclization: The Third Way**

Supplementary Information

Synthesis of Polycyclic Aromatic Hydrocarbons via Phenyl Addition – Dehydrocyclization: The Third Way

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Synthesis of 1-(2-bromophenyl)naphthalene

Materials and General Methods. Unless otherwise stated, all manipulations of air and/or moisture sensitive compounds were carried out in oven-dried glassware, under an atmosphere of nitrogen gas. All solvents and reagents were purchased from Alfa Aesar, Spectrum Chemicals, Acros Organics, TCI America, and Sigma-Aldrich and were used as received unless otherwise noted. Organic solvents were dried by passing through a column of alumina and were degassed by vigorous bubbling of nitrogen or argon through the solvent for 20 min. Flash column chromatography was performed on SiliCycle silica gel (particle size 40–63 μm). Thin layer chromatography was carried out using SiliCycle silica gel 60 Å F-254 precoated plates (0.25 mm thick) and visualized by UV absorption. All ^1H and ^{13}C NMR spectra were recorded on Bruker AVB-400 and AVQ-400 MHz spectrometers, and are referenced to residual solvent peaks (CDCl_3 ^1H NMR = 7.26 ppm, ^{13}C NMR = 77.16 ppm). ESI mass spectrometry was performed on a Finnigan LTQFT (Thermo) spectrometer in positive ionization mode.

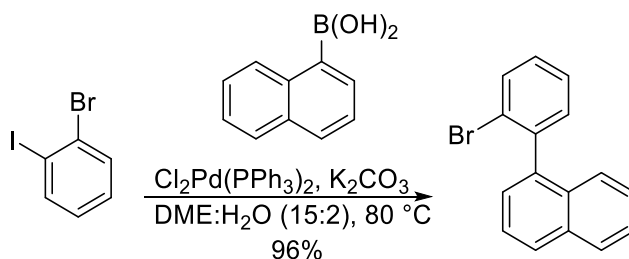


Figure S2. The synthesis of 1-(2-bromophenyl)naphthalene.

Procedure for 1-(2-bromophenyl)naphthalene: 2.0 g (7.07 mmol) of 1-bromo-2-iodobenzene, 1.34 g (7.78 mmol) of naphthalen-1-ylboronic acid, 2.44 g (17.67 mmol) K₂CO₃, 74.43 mg (0.11 mmol) of Cl₂Pd(PPh₃)₂ in a 30 ml mixture of DME:H₂O (15:2) were stirred at 80°C for four hours. After cooling, the product was extracted with diethyl ether (3 × 15 ml) and dried with sodium sulfate. After the solvent was removed, the residue was purified by silica gel column chromatography (hexane), yielding 1.92g (96%) of 1-(2-bromophenyl)naphthalene as a colorless solid. ^1H NMR (400 MHz, in CDCl_3): δ 7.92(d, J = 8.2 Hz, 2H), 7.75 (dd, J = 7.91 Hz, J = 1.03 Hz, 1H), 7.58 – 7.29 (m, 8H). ^{13}C NMR (101 MHz, in CDCl_3): δ 141.5, 139.2, 133.6, 132.8, 132.3, 131.7, 129.9, 129.5, 128.5, 128.2, 127.4, 126.9, 126.7, 126.5, 125.4, 124.5. HRMS (EI+) calcd. for C₁₆H₁₁Br 282.0044, found 282.0048.

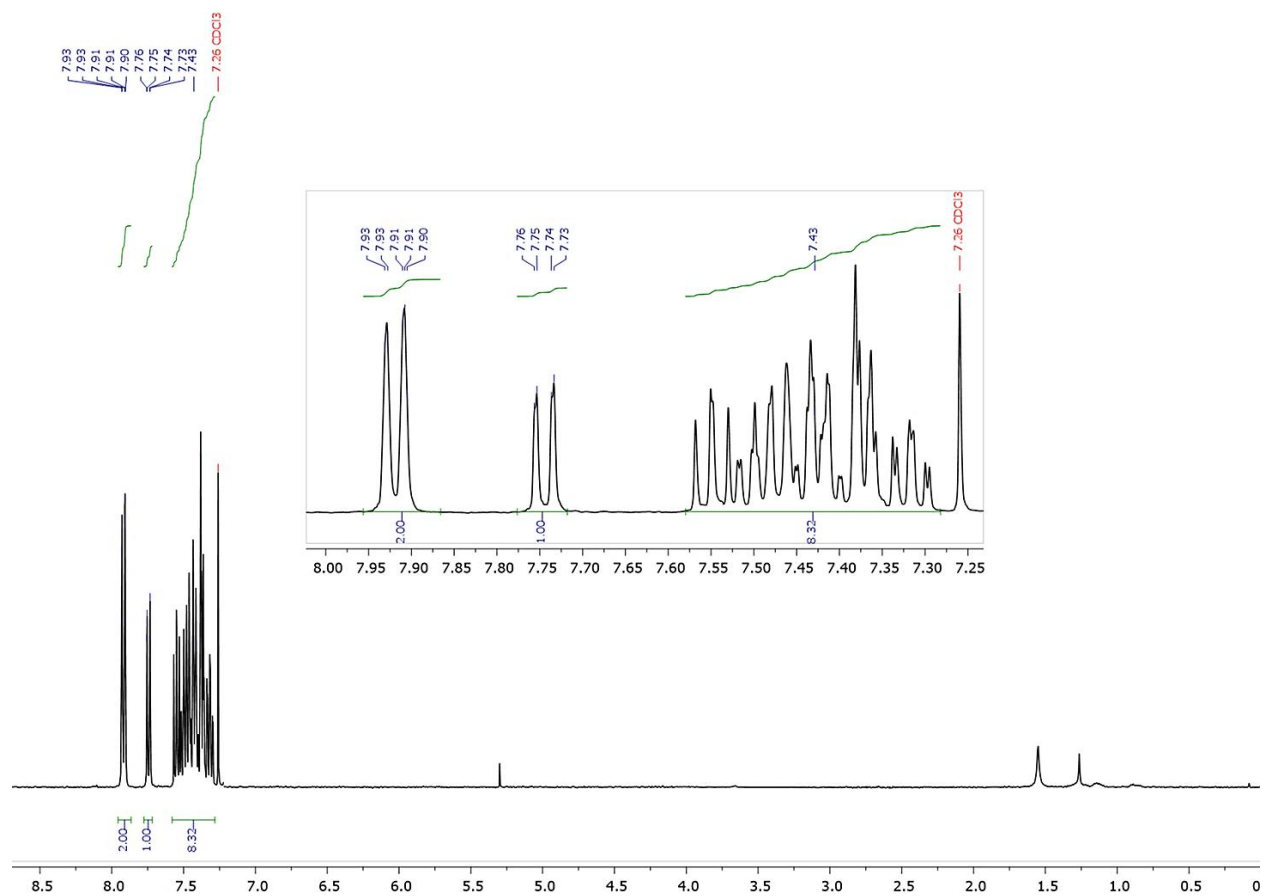


Figure S3. ^1H NMR spectrum of 1-(2-bromophenyl)naphthalene.

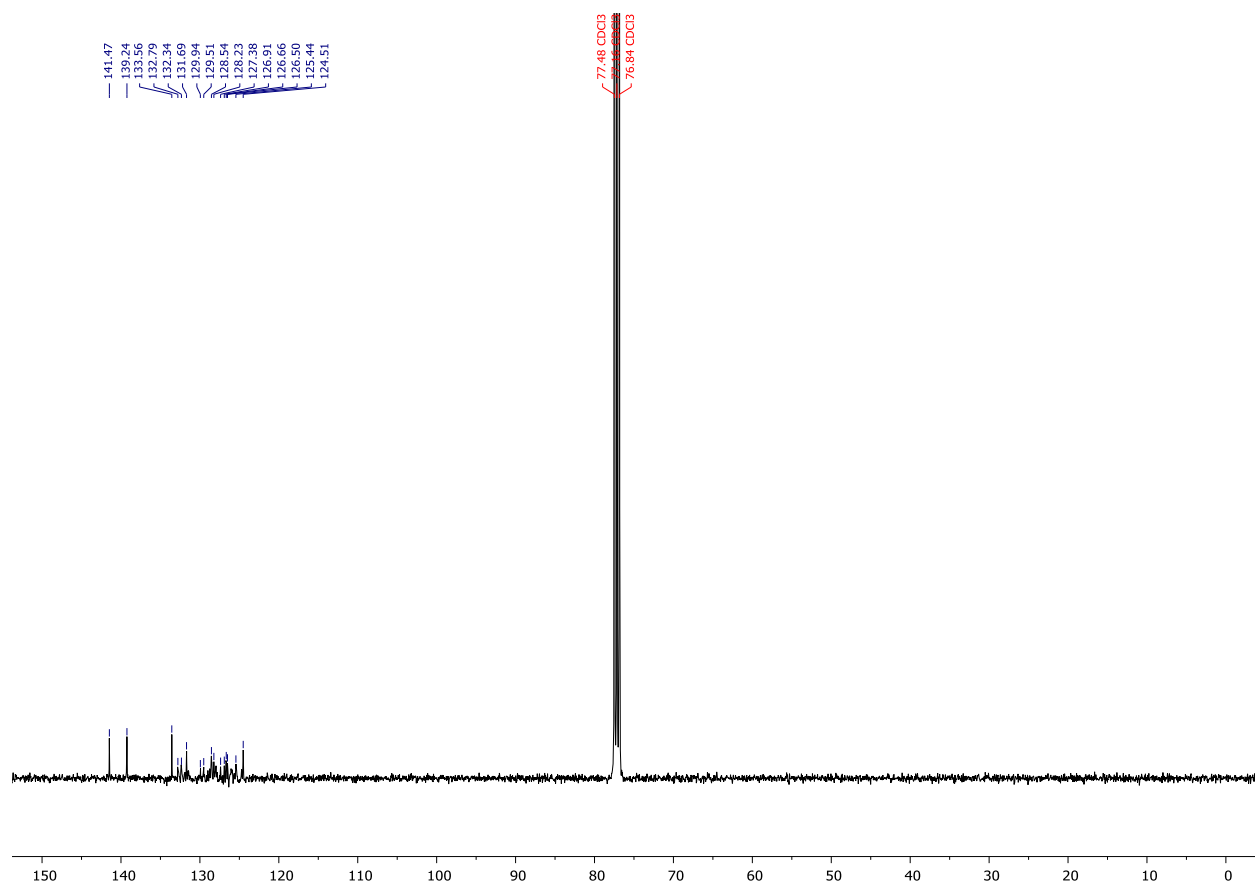


Figure S4. ¹³C NMR spectrum of 1-(2-bromophenyl)naphthalene.

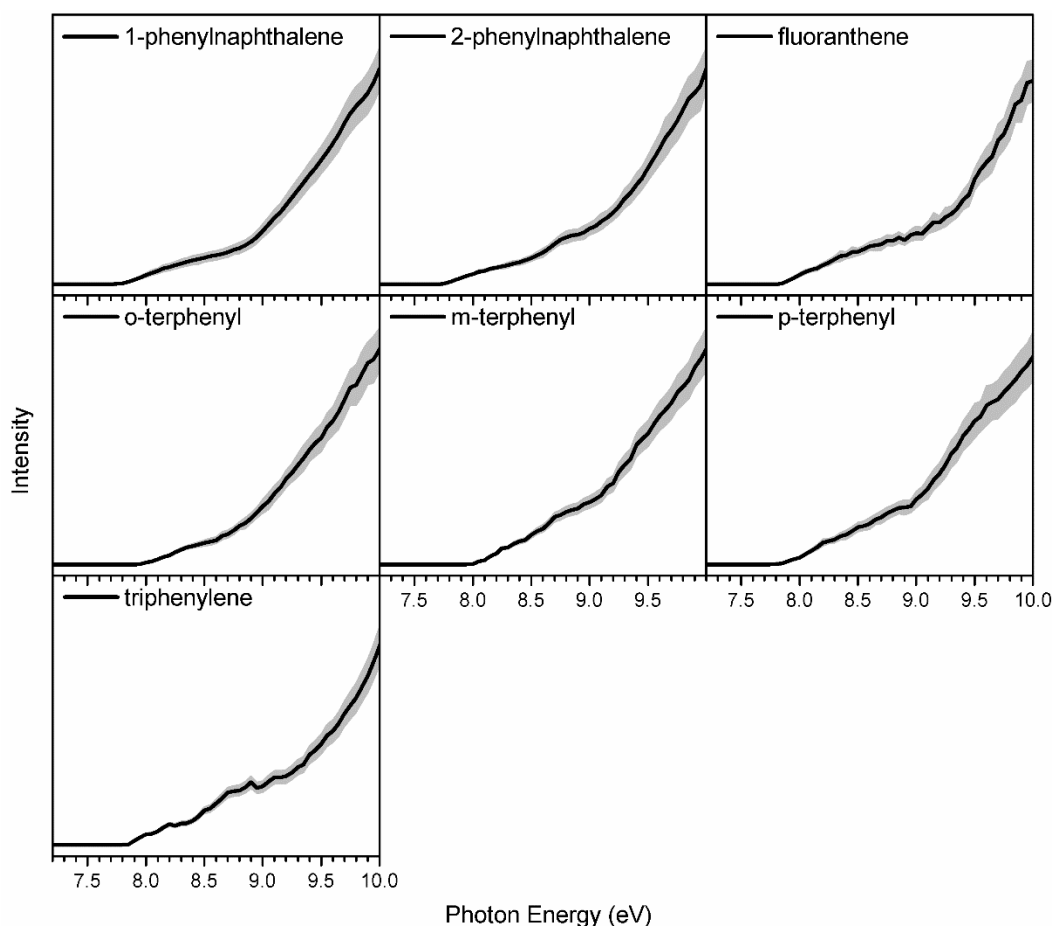


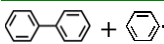

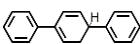
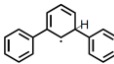

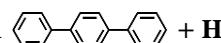
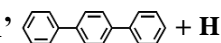
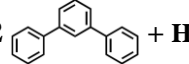

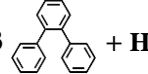

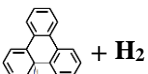
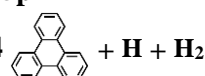
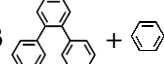


Figure S5. Calibration photoionization efficiency (PIE) curves recorded for helium-seeded 1-phenylnaphthalene, 2-phenylnaphthalene, fluoranthene, *o*-terphenyl, *m*-terphenyl, *p*-terphenyl and triphenylene at identical physical conditions (pressure, temperature) as the real experiments.

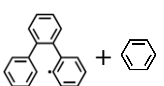

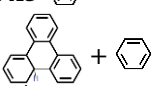
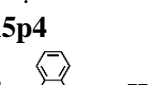
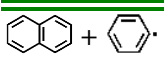
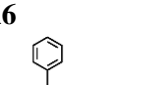
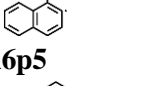
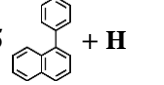
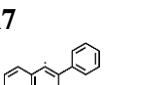
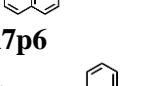
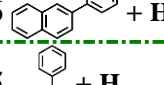
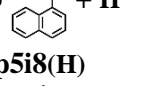
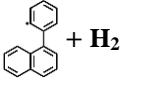

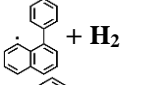

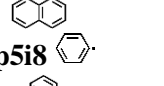
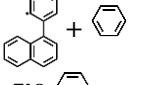
These PIE calibration curves were newly recorded and are shown as black lines along with the error limits (grey area). The adiabatic ionization energies of these isomers were determined to be 7.75 ± 0.05 , 7.70 ± 0.05 , 7.80 ± 0.05 , 7.95 ± 0.05 eV, 8.00 ± 0.05 eV, 7.80 ± 0.05 eV and 7.85 ± 0.05 eV, respectively, and are in excellent agreement with literature values of 7.75 eV,^[7] 7.90 ± 0.10 eV,^[8] 7.99 ± 0.01 eV,^[9] 8.01 ± 0.01 eV,^[9] 7.80 ± 0.03 eV,^[10] and 7.89 ± 0.04 eV^[11]. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans.


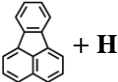


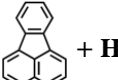
Table S1. Experiment conditions of the experiments.

Reaction	Temperature (K)	Pressure (atm)	Heating length (mm)	Inner diameter of the tube (mm)
Biphenyl / nitrosobenzene	1300 ± 10	0.394 ± 0.005	20	2
1-(2-Bromophenyl)naphthalene pyrolysis	1300 ± 10	0.394 ± 0.005	20	2
Naphthalene / nitrosobenzene	1100 ± 10	0.394 ± 0.005	20	2

Table S2. The CCSD(T)/cc-pVDZ energies on the B3LYP/cc-pVTZ optimized geometries of relevant reactants, intermediates, transition states and products on their adiabatic singlet or doublet ground state potential energy surfaces.

	B3LYP/ cc-pVTZ + E_{zpc} ^a	E_{zpc} ^b	CCSD(T)/cc- pVDZ	E^c (kJ/mol)
 + 	-694.841940	0.268593	-692.879086	0
tsi1	-694.831530	0.268777	-692.869142	27
tsi2	-694.830513	0.268698	-692.869009	27
tsi3	-694.830653	0.268960	-692.870947	22
i1 	-694.872055	0.271169	-692.924032	-111
i2 	-694.866879	0.270570	-692.922434	-109
i3 	-694.868276	0.270924	-692.922554	-108
tsi1p1	-694.829240	0.263908	-692.866755	20
tsi2p2	-694.827982	0.263848	-692.872553	5
tsi3p3	-694.823732	0.263820	-692.873105	3
p1  + H	-694.839788	0.262110	-692.888981	-43
p1'  + H	-694.839831	0.262102	-692.888954	-43
p2  + H	-694.839408	0.262012	-692.889123	-44
p3  + H	-694.833183	0.261860	-692.887213	-39
p3  + H	-694.833183	0.261860	-692.887213	0
tsp3i4 (H)	-694.815507	0.259667	-692.848384	96
i4  + H ₂	-694.825652	0.258790	-692.862287	58
tsi4i5 (H)	-694.820262	0.258139	-692.858247	67
i5  + H ₂	-694.863946	0.260012	-692.908436	-60
tsi5p4	-694.829826	0.253086	-692.864993	36
p4  + H + H ₂	-694.841292	0.251109	-692.880777	-11
p3  + 	-925.887893	0.349103	-923.282577	121
tsp3i4 	-925.873370	0.344141	-923.258289	172

i4		-925.888709	0.349100	-923.278432	132
tsi4i5		-925.883319	0.348449	-923.274392	141
i5		-925.927003	0.350322	-923.324582	14
tsi5p4		-925.892883	0.343396	-923.281139	110
p4		-925.904349	0.341419	-923.296923	63
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		-617.435192	0.234463	-615.685395	0
tsi6		-617.425997	0.234556	-615.677339	21
i6		-617.471509	0.237091	-615.740050	-137
tsi6p5		-617.419928	0.229844	-615.682746	-5
p5		-617.428559	0.228029	-615.693804	-39
tsi7		-617.425094	0.234621	-615.675936	25
i7		-617.465453	0.236878	-615.732144	-116
tsi7p6		-617.422363	0.229831	-615.681756	-3
p6		-617.432888	0.227980	-615.695420	-43
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p5		-617.428559	0.228029	-615.693804	0
tsp5i8(H)		-617.410660	0.225869	-615.653167	101
i8		-617.421067	0.224996	-615.664243	70
tsp5i9(H)		-617.408895	0.225943	-615.662622	76
i9		-617.422301	0.224968	-615.676171	38
p5		-848.483269	0.315272	-846.089167	121
tsp5i8		-848.468946	0.310426	-846.063092	177
i8		-848.484124	0.315306	-846.080388	144
tsp5i9		-848.465205	0.310419	-846.062988	177
i9		-848.485358	0.315278	-846.092317	113
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i8		-616.251137	0.214927	-614.500789	0
tsi8i10		-616.229692	0.213276	-614.481360	47

i10		-616.283290	0.215106	-614.542125	-108
tsi10p7		-616.239333	0.207922	-614.489802	11
p7		-616.247762	0.206308	-614.506544	-38
i9		-616.252371	0.214899	-614.512718	-32
tsi9i11		-616.233601	0.213639	-614.489079	27
i11		-616.278252	0.214770	-614.533992	-88
tsi11p7		-616.238721	0.207979	-614.485517	21
p7		-616.247762	0.206308	-614.506544	-38

^a B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

^b zero-point energy by B3LYP/cc-pVTZ in hartree.

^c relative energy by CCSD(T)/cc-pVDZ with B3LYP/cc-pVTZ zero-point energy correction.

Table S3. Coordinates of relevant reactants, intermediates and products in the biphenyl (C₁₂H₁₀) - phenyl (C₆H₅[•]) system.

biphenyl		phenyl	
C	-0.401663; 1.131029; -2.849995	C	0.000000; 1.221238; 0.769133
C	-0.401074; 1.130701; -1.461548	C	0.000000; 1.209128; -0.629799
C	0.000000; 0.000000; -0.741140	C	0.000000; 0.000000; -1.318515
C	0.401074; -1.130701; -1.461548	C	0.000000; -1.209128; -0.629799
C	0.401663; -1.131029; -2.849995	C	0.000000; -1.221238; 0.769133
C	0.000000; 0.000000; -3.551196	C	0.000000; 0.000000; 1.391403
H	-0.724520; 2.014386; -3.385092	H	0.000000; 2.153163; 1.318818
H	-0.738908; 2.009071; -0.928177	H	0.000000; 2.145567; -1.173412
H	0.738908; -2.009071; -0.928177	H	0.000000; 0.000000; -2.400146
H	0.724520; -2.014386; -3.385092	H	0.000000; -2.145567; -1.173412
H	0.000000; 0.000000; -4.632911	H	0.000000; -2.153163; 1.318818
C	0.000000; 0.000000; 0.741140		
C	0.401074; 1.130701; 1.461548		
C	-0.401074; -1.130701; 1.461548		
C	0.401663; 1.131029; 2.849995		
H	0.738908; 2.009071; 0.928177		
C	-0.401663; -1.131029; 2.849995		
H	-0.738908; -2.009071; 0.928177		
C	0.000000; 0.000000; 3.551196		
H	0.724520; 2.014386; 3.385092		
H	-0.724520; -2.014386; 3.385092		
H	0.000000; 0.000000; 4.632911		
i1		i2	
C	4.660616; 1.426712; 0.284173	C	-4.40781; -0.561817; 1.172172
C	3.318839; 1.157142; 0.498834	C	-3.210045; 0.132842; 1.064994
C	2.727042; -0.037311; 0.04249	C	-2.410817; 0.018962; -0.077481
C	3.562205; -0.944578; -0.639115	C	-2.857664; -0.807696; -1.113468
C	4.904349; -0.67348; -0.849286	C	-4.055789; -1.501657; -1.008225
C	5.465736; 0.51434; -0.390808	C	-4.836348; -1.382926; 0.135811
H	5.079835; 2.359189; 0.639007	H	-5.004352; -0.46548; 2.069833
H	2.712537; 1.897291; 1.001081	H	-2.878909; 0.754265; 1.886276
H	3.16121; -1.887984; -0.980975	H	-2.269934; -0.88935; -2.017856
H	5.519205; -1.397883; -1.367313	H	-4.384457; -2.129751; -1.82583
H	6.513405; 0.725379; -0.556528	H	-5.770202; -1.922768; 0.217608
C	1.314705; -0.32249; 0.265576	C	-1.123733; 0.754157; -0.184079
C	0.591282; -1.232946; -0.566082	C	-0.021305; 0.158123; -0.730523
C	0.579896; 0.296627; 1.32419	C	-1.030291; 2.089482; 0.297288
C	-0.719839; -1.510968; -0.38186	C	1.30979; 0.840718; -0.881685
H	1.100897; -1.692924; -1.401886	H	-0.073959; -0.870729; -1.061575
C	-0.727876; 0.040057; 1.556455	C	0.190659; 2.792458; 0.22047
H	1.096312; 0.973439; 1.99128	H	-1.905927; 2.575845; 0.701332
C	-1.542014; -0.906242; 0.720584	C	1.305403; 2.235376; -0.321823

H	-1.228508; -2.186751; -1.057467	H	0.233874; 3.805505; 0.601252
H	-1.233781; 0.520683; 2.384063	H	2.233062; 2.790375; -0.369126
H	-1.887117; -1.722806; 1.375148	H	1.52735; 0.91472; -1.961158
C	-2.820652; -0.250239; 0.188838	C	2.452033; -0.003392; -0.305111
C	-2.74818; 0.838262; -0.681705	C	3.481561; -0.466705; -1.120535
C	-4.075818; -0.725207; 0.56153	C	2.47917; -0.321589; 1.053554
C	-3.903958; 1.435513; -1.166413	C	4.517702; -1.232486; -0.594951
H	-1.779211; 1.217541; -0.97949	H	3.473627; -0.22778; -2.1772
C	-5.236336; -0.129037; 0.077907	C	3.510976; -1.085766; 1.581451
H	-4.147812; -1.569495; 1.236535	H	1.684929; 0.032033; 1.698239
C	-5.153275; 0.953526; -0.78787	C	4.534903; -1.54428; 0.758092
H	-3.830679; 2.27863; -1.840848	H	5.309028; -1.584425; -1.243776
H	-6.20294; -0.511596; 0.378441	H	3.516799; -1.325179; 2.636786
H	-6.053686; 1.419216; -1.165669	H	5.338704; -2.140113; 1.169496
i3		<i>p</i>-terphenyl (D₂, P1)	
C	-3.663173; -0.644102; 0.907197	C	-0.001319; 1.195498; -0.692982
C	-2.61939; 0.265879; 0.895028	C	0.000000; 0.000000; -1.419085
C	-1.626329; 0.233494; -0.102093	C	0.001319; -1.195498; -0.692982
C	-1.73031; -0.778235; -1.071969	C	-0.001319; -1.195498; 0.692982
C	-2.779248; -1.686129; -1.062245	C	0.000000; 0.000000; 1.419085
C	-3.754712; -1.626103; -0.07482	C	0.001319; 1.195498; 0.692982
H	-4.404122; -0.59475; 1.694412	H	0.012949; 2.139714; -1.220795
H	-2.556176; 0.996583; 1.688752	H	-0.012949; -2.139714; -1.220795
H	-0.991807; -0.851334; -1.856317	H	0.012949; -2.139714; 1.220795
H	-2.832651; -2.445567; -1.831277	H	-0.012949; 2.139714; 1.220795
H	-4.568719; -2.338175; -0.063781	C	0.000000; 0.000000; 2.899875
C	-0.537162; 1.216231; -0.128929	C	0.755352; 0.932215; 3.620461
C	0.761874; 0.864711; -0.837548	C	-0.755352; -0.932215; 3.620461
C	-0.679035; 2.460745; 0.450229	C	0.756259; 0.932108; 5.008806
C	1.744688; 2.006158; -0.889828	H	1.367195; 1.647446; 3.087316
C	0.313772; 3.443931; 0.405982	C	-0.756259; -0.932108; 5.008806
H	-1.616034; 2.709898; 0.929758	H	-1.367195; -1.647446; 3.087316
C	1.527166; 3.195847; -0.283875	C	0.000000; 0.000000; 5.710205
H	2.668394; 1.817962; -1.421401	H	1.355675; 1.656997; 5.543743
H	0.140765; 4.403763; 0.871427	H	-1.355675; -1.656997; 5.543743
H	2.280017; 3.972234; -0.334121	H	0.000000; 0.000000; 6.791920
H	0.526925; 0.594361; -1.877183	C	0.000000; 0.000000; -2.899875
C	1.464848; -0.365562; -0.243391	C	0.755352; -0.932215; -3.620461
C	1.647907; -0.486809; 1.133807	C	-0.755352; 0.932215; -3.620461
C	1.98559; -1.354193; -1.075508	C	0.756259; -0.932108; -5.008806
C	2.327186; -1.575485; 1.664736	H	1.367195; -1.647446; -3.087316
H	1.253185; 0.274838; 1.793272	C	-0.756259; 0.932108; -5.008806
C	2.669; -2.444321; -0.547832	H	-1.367195; 1.647446; -3.087316
H	1.853011; -1.274419; -2.148065	C	0.000000; 0.000000; -5.710205
C	2.840734; -2.558849; 0.825781	H	1.355675; -1.656997; -5.543743
H	2.45605; -1.656659; 2.736119	H	-1.355675; 1.656997; -5.543743

H	3.062336; -3.204489; -1.21001	H	0.000000; 0.000000; -6.791920
H	3.368394; -3.407501; 1.240076		
<i>p</i>-terphenyl (C_{2h}, P1)			<i>m</i>-terphenyl (P2)
C	0.000000; 1.195528; 0.692941	C	0.064517; -0.030412; 0.000000
C	0.000000; 0.000000; 1.419372	C	0.729897; -0.158053; 1.222050
C	0.000000; -1.195528; 0.692941	C	2.103027; -0.423644; 1.204887
C	0.000000; -1.195528; -0.692941	C	2.778553; -0.555585; 0.000000
C	0.000000; 0.000000; -1.419372	C	2.103027; -0.423644; -1.204887
C	0.000000; 1.195528; -0.692941	C	0.729897; -0.158053; -1.222050
H	0.034462; 2.139483; 1.220196	H	-0.987202; 0.221216; 0.000000
H	-0.034462; -2.139483; 1.220196	H	2.635945; -0.552217; 2.137015
H	-0.034462; -2.139483; -1.220196	H	3.837329; -0.778996; 0.000000
H	0.034462; 2.139483; -1.220196	H	2.635945; -0.552217; -2.137015
C	0.000000; 0.000000; -2.900092	C	0.000322; -0.004472; -2.503810
C	-0.741598; 0.943153; -3.620898	C	0.582306; 0.665435; -3.585809
C	0.741598; -0.943153; -3.620898	C	-1.287976; -0.525214; -2.668248
C	-0.742169; 0.943274; -5.009201	C	-0.098454; 0.810491; -4.787109
H	-1.343084; 1.667192; -3.087940	H	1.567628; 1.098064; -3.475832
C	0.742169; -0.943274; -5.009201	C	-1.969225; -0.381658; -3.869519
H	1.343084; -1.667192; -3.087940	H	-1.749847; -1.068733; -1.855033
C	0.000000; 0.000000; -5.710487	C	-1.377697; 0.287158; -4.934887
H	-1.330452; 1.677081; -5.544304	H	0.368539; 1.340579; -5.606728
H	1.330452; -1.677081; -5.544304	H	-2.961271; -0.800445; -3.976041
H	0.000000; 0.000000; -6.792189	H	-1.908461; 0.399383; -5.870742
C	0.000000; 0.000000; 2.900092	C	0.000322; -0.004472; 2.503810
C	0.741598; -0.943153; 3.620898	C	-1.287976; -0.525214; 2.668248
C	-0.741598; 0.943153; 3.620898	C	0.582306; 0.665435; 3.585809
C	0.742169; -0.943274; 5.009201	C	-1.969225; -0.381658; 3.869519
H	1.343084; -1.667192; 3.087940	H	-1.749847; -1.068733; 1.855033
C	-0.742169; 0.943274; 5.009201	C	-0.098454; 0.810491; 4.787109
H	-1.343084; 1.667192; 3.087940	H	1.567628; 1.098064; 3.475832
C	0.000000; 0.000000; 5.710487	C	-1.377697; 0.287158; 4.934887
H	1.330452; -1.677081; 5.544304	H	-2.961271; -0.800445; 3.976041
H	-1.330452; 1.677081; 5.544304	H	0.368539; 1.340579; 5.606728
H	0.000000; 0.000000; 6.792189	H	-1.908461; 0.399383; 5.870742
<i>o</i>-terphenyl (P3)			i4
C	-0.029430; 0.704710; 1.199074	C	-0.588382; 1.259342; -0.013139
C	0.029430; -0.704710; 1.199074	C	0.817546; 1.14985; 0.021287
C	0.070388; -1.374862; 2.427175	C	1.583177; 2.32111; 0.040564
C	0.038615; -0.693062; 3.634193	C	0.99568; 3.576896; 0.03163
C	-0.038615; 0.693062; 3.634193	C	-0.388034; 3.684952; 0.010565
C	-0.070388; 1.374862; 2.427175	C	-1.162606; 2.53417; -0.010825
H	0.097653; -2.456353; 2.425493	H	2.659986; 2.239777; 0.099533
H	0.064269; -1.242017; 4.566029	H	1.615588; 4.463126; 0.054933
H	-0.064269; 1.242017; 4.566029	H	-0.863201; 4.656776; 0.006549
H	-0.097653; 2.456353; 2.425493	H	-2.2406; 2.615782; -0.051208

C	-0.008270; 1.527460; -0.041531	C	-1.499569; 0.084347; -0.086643
C	1.002721; 1.381364; -0.996030	C	-2.502105; -0.092747; 0.87103
C	-0.976025; 2.515021; -0.249364	C	-1.425117; -0.825794; -1.145751
C	1.042956; 2.194500; -2.120348	C	-3.395961; -1.152657; 0.780284
H	1.767691; 0.631340; -0.850806	H	-2.57018; 0.598563; 1.700703
C	-0.940511; 3.325290; -1.377684	C	-2.321555; -1.881014; -1.240611
H	-1.770955; 2.638898; 0.474521	H	-0.66402; -0.698804; -1.903517
C	0.070388; 3.168554; -2.317858	C	-3.309258; -2.050687; -0.276389
H	1.838518; 2.068623; -2.842874	H	-4.158944; -1.276992; 1.537465
H	-1.704876; 4.077541; -1.522028	H	-2.250958; -2.570422; -2.071607
H	0.101271; 3.799458; -3.196098	H	-4.006121; -2.874936; -0.349754
C	0.008270; -1.527460; -0.041531	C	1.517717; -0.156964; 0.092469
C	0.976025; -2.515021; -0.249364	C	2.715865; -0.401271; -0.603646
C	-1.002721; -1.381364; -0.996030	C	1.080736; -1.208563; 0.869394
C	0.940511; -3.325290; -1.377684	C	3.380455; -1.616703; -0.488051
H	1.770955; -2.638898; 0.474521	H	3.113271; 0.367281; -1.254779
C	-1.042956; -2.194500; -2.120348	C	1.687405; -2.424011; 1.025578
H	-1.767691; -0.631340; -0.850806	C	2.879561; -2.629527; 0.322892
C	-0.070388; -3.168554; -2.317858	H	4.295549; -1.775725; -1.042634
H	1.704876; -4.077541; -1.522028	H	1.273461; -3.195625; 1.661498
H	-1.838518; -2.068623; -2.842874	H	3.402831; -3.573182; 0.40899
H	-0.101271; -3.799458; -3.196098		
i5		triphenylene (P4)	
C	-1.204529; 0.861705; -0.004233	C	0.707680; 1.252902; 0.000000
C	-1.362988; -0.542399; 0.105518	C	-0.707680; 1.252902; 0.000000
C	-2.655381; -1.065694; 0.215532	C	-1.378272; 2.491214; 0.000000
C	-3.772656; -0.247209; 0.181233	C	-0.697568; 3.688465; 0.000000
C	-3.61866; 1.12952; 0.032853	C	0.697568; 3.688465; 0.000000
C	-2.349765; 1.672214; -0.052739	C	1.378272; 2.491214; 0.000000
H	-2.79182; -2.130722; 0.338208	H	-2.456541; 2.519524; 0.000000
H	-4.76003; -0.678462; 0.276822	H	-1.245409; 4.621173; 0.000000
H	-4.485578; 1.776241; 0.011164	H	1.245409; 4.621173; 0.000000
H	-2.234127; 2.745333; -0.116479	H	2.456541; 2.519524; 0.000000
C	0.137236; 1.420047; -0.024431	C	1.438885; -0.013583; 0.000000
C	0.459593; 2.62592; -0.607294	C	2.846591; -0.051989; 0.000000
C	1.190956; 0.601301; 0.686185	C	0.731205; -1.239320; 0.000000
C	1.759077; 3.137804; -0.589064	C	3.543088; -1.240121; 0.000000
H	-0.31181; 3.184042; -1.122283	H	3.410242; 0.867665; 0.000000
C	2.558714; 1.213515; 0.635812	C	1.468319; -2.439225; 0.000000
C	2.797509; 2.408945; 0.046602	C	2.845520; -2.448344; 0.000000
H	1.977052; 4.078853; -1.073333	H	4.624758; -1.232031; 0.000000
H	3.361609; 0.692228; 1.138056	H	0.953701; -3.387189; 0.000000
H	3.799734; 2.818691; 0.055523	H	3.379349; -3.389142; 0.000000
C	-0.17127; -1.409144; 0.02045	C	-1.438885; -0.013583; 0.000000
C	-0.268829; -2.756652; -0.346234	C	-2.846591; -0.051989; 0.000000
C	1.105749; -0.866629; 0.256159	C	-0.731205; -1.239320; 0.000000

C	0.856829; -3.557905; -0.455938	C	-3.543088; -1.240121; 0.000000
H	-1.236119; -3.180191; -0.575542	H	-3.410242; 0.867665; 0.000000
C	2.229523; -1.676169; 0.130198	C	-1.468319; -2.439225; 0.000000
C	2.112594; -3.016699; -0.217367	C	-2.845520; -2.448344; 0.000000
H	0.753807; -4.595587; -0.743841	H	-4.624758; -1.232031; 0.000000
H	3.213746; -1.261778; 0.291462	H	-0.953701; -3.387189; 0.000000
H	2.999947; -3.628071; -0.313108	H	-3.379349; -3.389142; 0.000000
H	0.891373; 0.584607; 1.753898		

Table S4. Coordinates of relevant reactants, intermediates and products in the naphthalene (C₁₀H₈) - phenyl (C₆H₅[•]) system.

naphthalene		i6	
C	0.000000; 2.423896; 0.705848	C	3.230301; -1.785215; 0.344279
C	0.000000; 1.240661; 1.396932	C	3.26188; -0.42499; 0.579152
C	0.000000; 0.000000; 0.713987	C	2.194027; 0.408507; 0.189884
C	0.000000; 0.000000; -0.713987	C	1.069611; -0.174843; -0.442463
C	0.000000; 1.240661; -1.396932	C	1.05971; -1.546479; -0.671595
C	0.000000; 2.423896; -0.705848	C	2.124553; -2.352597; -0.288628
H	0.000000; -1.239240; 2.479812	H	3.10563; 2.242863; 0.905605
H	0.000000; 3.364555; 1.240263	H	4.061; -2.407762; 0.649139
H	0.000000; 1.239240; 2.479812	H	4.119187; 0.02264; 1.066389
C	0.000000; -1.240661; 1.396932	C	2.238811; 1.819701; 0.416596
C	0.000000; -1.240661; -1.396932	C	-0.111697; 0.679142; -0.889608
H	0.000000; 1.239240; -2.479812	H	0.19903; -1.995554; -1.151308
H	0.000000; 3.364555; -1.240263	H	2.092073; -3.41685; -0.479028
C	0.000000; -2.423896; -0.705848	C	0.076989; 2.144456; -0.612946
C	0.000000; -2.423896; 0.705848	C	1.185419; 2.645859; 0.006796
H	0.000000; -1.239240; -2.479812	H	-0.203048; 0.559667; -1.978461
H	0.000000; -3.364555; -1.240263	H	-0.724938; 2.80328; -0.918487
H	0.000000; -3.364555; 1.240263	H	1.253509; 3.711843; 0.18584
		C	-1.445449; 0.196138; -0.311872
		C	-1.650505; 0.158887; 1.068634
		C	-2.487259; -0.191214; -1.15115
		C	-2.864864; -0.260255; 1.59333
		H	-0.851466; 0.457807; 1.734616
		C	-3.707359; -0.610722; -0.628551
		H	-2.344562; -0.166136; -2.224754
		C	-3.899225; -0.646921; 0.745771
		H	-3.006194; -0.285433; 2.66592
		H	-4.50429; -0.909488; -1.296887
		H	-4.845581; -0.973603; 1.155649
i7		1-phenylnaphthalene (P5)	
C	-4.29878; -0.276594; -0.596533	C	3.309639; -1.827228; 0.222462
C	-3.434908; 0.809554; -0.679861	C	3.479399; -0.480289; 0.04446
C	-2.145002; 0.746218; -0.162348	C	2.367077; 0.391884; -0.046361
C	-1.694402; -0.461365; 0.470142	C	1.045556; -0.151147; 0.031741
C	-2.599214; -1.556354; 0.537685	C	0.911165; -1.54832; 0.235927
C	-3.869982; -1.461879; 0.016919	C	2.010205; -2.362908; 0.327642
H	-1.576845; 2.768155; -0.723758	H	3.54492; 2.186061; -0.258619
H	-5.29801; -0.207504; -1.003986	H	4.168935; -2.480791; 0.292344
H	-3.76507; 1.725313; -1.155123	H	4.473995; -0.057518; -0.023241
C	-1.226368; 1.863201; -0.241017	C	2.539992; 1.787916; -0.197667
C	-0.404559; -0.533076; 0.993164	C	-0.074454; 0.735694; -0.063747
H	-2.269992; -2.472941; 1.010687	H	-0.077044; -1.972756; 0.331587


H	-4.542568; -2.307079; 0.081259	H	1.880194; -3.424964; 0.488164
C	0.578815; 0.596453; 0.941179	C	0.152444; 2.089435; -0.192012
C	0.016326; 1.81197; 0.254154	C	1.455152; 2.619255; -0.259253
H	-0.075922; -1.451581; 1.46329	H	-0.694453; 2.758324; -0.268811
H	0.822725; 0.885673; 1.976489	H	1.589718; 3.686846; -0.371497
H	0.672846; 2.668976; 0.171277	C	-1.477911; 0.241945; -0.032149
C	1.912365; 0.159675; 0.323694	C	-2.368152; 0.706289; 0.940357
C	1.977783; -0.234097; -1.013817	C	-1.956161; -0.654076; -0.993994
C	3.079451; 0.140995; 1.083522	C	-3.692851; 0.286229; 0.954954
C	3.182143; -0.635372; -1.575667	H	-2.012455; 1.393119; 1.696962
H	1.078538; -0.224105; -1.61609	C	-3.280914; -1.070905; -0.982832
C	4.288263; -0.26154; 0.523936	H	-1.287622; -1.011519; -1.765687
H	3.044077; 0.444098; 2.123	C	-4.154292; -0.604139; -0.006703
C	4.342729; -0.65088; -0.807858	H	-4.363283; 0.653563; 1.720755
H	3.216236; -0.936825; -2.614431	H	-3.632759; -1.757334; -1.741729
H	5.185011; -0.269655; 1.129568	H	-5.18551; -0.930835; 0.002823
H	5.281017; -0.963988; -1.245942		
2-phenylnaphthalene (P6)		i8	
C	4.558982; -0.066477; 0.034751	C	3.330788; -1.803933; 0.203703
C	3.692102; 0.974825; -0.173494	C	3.482574; -0.452707; 0.04391
C	2.292489; 0.769771; -0.140681	C	2.358872; 0.404892; -0.043409
C	1.79059; -0.542093; 0.108992	C	1.043648; -0.155291; 0.024022
C	2.713824; -1.595385; 0.323185	C	0.928818; -1.556022; 0.207681
C	4.064037; -1.364348; 0.286284	C	2.03823; -2.357503; 0.292414
H	1.733161; 2.813511; -0.547438	H	3.519143; 2.211555; -0.243584
H	5.627186; 0.102534; 0.008121	H	4.19841; -2.446802; 0.269611
H	4.069338; 1.971539; -0.365501	H	4.471251; -0.015107; -0.014872
C	1.361937; 1.816204; -0.346727	C	2.518071; 1.803024; -0.189258
C	0.392461; -0.748382; 0.141347	C	-0.08558; 0.722051; -0.06904
H	2.333986; -2.590891; 0.51614	H	-0.05334; -1.997324; 0.286288
H	4.757897; -2.178099; 0.450131	H	1.92055; -3.423632; 0.434036
C	-0.501573; 0.281374; -0.061063	C	0.12911; 2.078262; -0.202571
C	0.014747; 1.582391; -0.306384	C	1.425019; 2.622441; -0.261348
H	0.026318; -1.744069; 0.356966	H	-0.721878; 2.739252; -0.295332
H	-0.674554; 2.395295; -0.489761	H	1.548008; 3.690968; -0.377022
C	-1.964644; 0.050351; -0.022699	C	-1.482846; 0.222739; -0.034863
C	-2.526108; -1.11333; -0.561219	C	-2.475161; 0.868756; 0.727366
C	-2.826524; 0.989104; 0.555679	C	-1.936497; -0.859822; -0.758592
C	-3.896124; -1.332605; -0.518067	C	-3.79376; 0.430668; 0.715938
H	-1.884287; -1.840304; -1.040284	H	-2.193601; 1.712177; 1.344987
C	-4.196902; 0.769877; 0.600438	C	-3.217095; -1.338877; -0.813947
H	-2.417321; 1.887825; 0.997276	C	-4.175669; -0.66584; -0.049794
C	-4.738625; -0.39214; 0.063782	H	-4.52932; 0.947487; 1.317619
H	-4.3075; -2.236111; -0.948548	H	-3.485733; -2.194003; -1.420411
H	-4.841878; 1.506218; 1.061594	H	-5.204619; -1.001588; -0.054582
H	-5.806357; -0.562257; 0.09657		

i9		i10	
C	3.270455; -1.86446; 0.259741	C	-2.107272; 2.400836; -0.313461
C	3.460284; -0.518075; 0.090055	C	-2.911777; 1.263017; -0.099092
C	2.368529; 0.378944; -0.029739	C	-2.296432; -0.017299; 0.097377
C	1.027707; -0.138053; 0.019407	C	-0.911917; -0.023684; 0.263626
C	0.934766; -1.519091; 0.204502	C	-0.087987; 1.207257; 0.462605
C	1.955396; -2.397015; 0.321329	C	-0.741839; 2.403971; -0.158266
H	3.562232; 2.165079; -0.218492	H	-3.990464; -1.33958; -0.153484
H	4.118967; -2.530366; 0.351066	H	-3.983525; 1.331555; -0.227637
H	4.463624; -0.113925; 0.048962	C	-2.916347; -1.276798; -0.033994
C	2.55384; 1.772807; -0.180485	C	-0.12469; -1.158965; 0.122918
C	-0.085553; 0.751419; -0.087018	H	-0.165034; 3.29774; -0.353475
H	1.796084; -3.458522; 0.459501	C	-0.750205; -2.397856; -0.022653
C	0.163807; 2.100929; -0.225276	C	-2.147934; -2.435574; -0.065608
C	1.474934; 2.611133; -0.272319	H	-0.180403; -3.311637; -0.12532
H	-0.669381; 2.783277; -0.324671	H	-2.644345; -3.391057; -0.17356
H	1.623672; 3.676189; -0.390472	C	2.513031; 1.375289; 0.083718
C	-1.478762; 0.244963; -0.046297	C	1.311151; 0.695909; 0.160229
C	-2.445218; 0.894536; 0.729655	C	1.275995; -0.712522; 0.058126
C	-1.87156; -0.872899; -0.790678	C	2.45395; -1.428903; -0.118799
C	-3.757462; 0.442074; 0.763089	C	3.658627; -0.737314; -0.207608
H	-2.157534; 1.74709; 1.330165	C	3.6893; 0.65126; -0.11365
C	-3.184793; -1.323589; -0.759624	H	2.548529; 2.454115; 0.16874
C	-4.133129; -0.669614; 0.018008	H	2.439189; -2.508413; -0.194761
H	-4.485307; 0.954063; 1.378661	H	4.580684; -1.28384; -0.354579
H	-3.468215; -2.184785; -1.350169	H	4.633489; 1.173376; -0.192485
H	-5.155104; -1.023354; 0.043969	H	-2.593737; 3.312303; -0.638847
H	-1.148485; -1.378791; -1.414619	H	-0.078309; 1.4137; 1.5526
i11		fluoranthene (P7)	
C	-2.171103; -2.409906; 0.092462	C	0.000000; 2.420049; 2.156911
C	-2.919603; -1.256325; 0.179724	C	0.000000; 1.274613; 2.923832
C	-2.289949; 0.010665; 0.089708	C	0.000000; 0.000000; 2.298836
C	-0.896453; -0.000402; -0.087087	C	0.000000; 0.000000; 0.901141
C	-0.133573; -1.176301; -0.187808	C	0.000000; 1.167991; 0.105743
C	-0.766862; -2.39038; -0.10145	C	0.000000; 2.387952; 0.738907
H	-3.97384; 1.364437; 0.300147	H	0.000000; -1.346736; 4.003981
H	-3.990917; -1.315475; 0.323686	H	0.000000; 1.346736; 4.003981
C	-2.902049; 1.287943; 0.169775	C	0.000000; -1.274613; 2.923832
C	-0.098154; 1.17481; -0.159844	C	0.000000; -1.167991; 0.105743
H	-0.226108; -3.324891; -0.177452	H	0.000000; 3.318850; 0.186674
C	-0.733816; 2.405194; -0.073543	C	0.000000; -2.387952; 0.738907
C	-2.133707; 2.434944; 0.084558	C	0.000000; -2.420049; 2.156911
H	-0.180497; 3.333337; -0.124798	H	0.000000; -3.318850; 0.186674
H	-2.625341; 3.397248; 0.147359	H	0.000000; -3.382828; 2.650918
C	2.49074; -1.422418; 0.12589	C	0.000000; 1.408818; -2.491764
C	1.296945; -0.755451; -0.481347	C	0.000000; 0.711123; -1.294332

C	1.273768; 0.751797; -0.256511	C	0.000000; -0.711123; -1.294332
C	2.454635; 1.433394; -0.039025	C	0.000000; -1.408818; -2.491764
C	3.6319; 0.725717; 0.20127	C	0.000000; -0.696037; -3.690468
C	3.608429; -0.693604; 0.362198	C	0.000000; 0.696037; -3.690468
H	2.478875; -2.493961; 0.275555	H	0.000000; -2.491145; -2.503495
H	2.454464; 2.513388; 0.045054	H	0.000000; -1.230609; -4.630979
H	4.552568; 1.261523; 0.385369	H	0.000000; 1.230609; -4.630979
H	4.504619; -1.186889; 0.71685	H	0.000000; 2.491145; -2.503495
H	-2.669281; -3.367533; 0.170776	H	0.000000; 3.382828; 2.650918
H	1.408556; -0.89924; -1.576383		

Table S5. Coordinates of relevant transition states.



Atom	X	Y	Z	Atom	X	Y	Z
tsi2				tsi2p2			
C	-4.730332	-0.324253	0.259982	C	4.839427	-0.250228	0.547797
C	-3.614261	0.498278	0.185395	C	3.64696	0.459805	0.592068
C	-2.343605	-0.032641	-0.062503	C	2.501044	-0.01788	-0.052668
C	-2.229094	-1.416816	-0.23169	C	2.590452	-1.229689	-0.745895
C	-3.344678	-2.240233	-0.15586	C	3.783163	-1.939018	-0.792348
C	-4.600655	-1.69789	0.090061	C	4.913232	-1.452902	-0.145112
H	-5.704338	0.109882	0.443771	H	5.7106	0.133761	1.061975
H	-3.73153	1.567951	0.296458	H	3.596139	1.383131	1.153411
H	-1.253349	-1.852535	-0.399805	H	1.724408	-1.606924	-1.273014
H	-3.230664	-3.309021	-0.280689	H	3.831387	-2.869685	-1.34216
H	-5.469811	-2.339183	0.149219	H	5.842315	-2.00572	-0.180729
C	-1.151687	0.845593	-0.143371	C	1.227866	0.74179	-0.000253
C	-0.165382	0.623893	-1.097871	C	0.011951	0.083272	0.144915
C	-1.002408	1.934525	0.731438	C	1.221346	2.138841	-0.117897
C	0.999574	1.422564	-1.152408	C	-1.214646	0.785084	0.241282
H	-0.281424	-0.182392	-1.809008	H	-0.002874	-0.994002	0.231434
C	0.097001	2.786571	0.628684	C	0.020566	2.842639	-0.125272
H	-1.747601	2.112571	1.494376	H	2.153779	2.66812	-0.256827
C	1.0768	2.561964	-0.318733	C	-1.184593	2.184667	0.019244
H	0.175391	3.636928	1.293672	H	0.032131	3.916766	-0.255234
H	1.920271	3.232757	-0.406366	H	-2.111026	2.7415	0.029016
H	1.61485	1.382138	-2.040286	H	-1.253284	0.920507	2.011771
C	2.545333	0.066878	-0.305666	C	-2.499682	0.024401	0.155569
C	3.376404	-0.584391	-1.189219	C	-2.724239	-1.110306	0.940213
C	2.596876	-0.110826	1.058293	C	-3.492046	0.412059	-0.747197
C	4.324573	-1.468854	-0.668947	C	-3.902121	-1.834659	0.825088
H	3.309222	-0.425127	-2.259192	H	-1.978616	-1.410545	1.664344
C	3.546539	-0.99843	1.56707	C	-4.674802	-0.30992	-0.860138
H	1.926389	0.421434	1.721132	H	-3.330121	1.272066	-1.382586
C	4.406125	-1.672801	0.704395	C	-4.884495	-1.43639	-0.07555
H	4.995055	-1.99474	-1.3374	H	-4.058185	-2.705784	1.447563
H	3.613833	-1.16055	2.635749	H	-5.428649	0.00632	-1.568961
H	5.140952	-2.358894	1.104076	H	-5.804294	-1.998915	-0.163076
tsi1				tsi1p1			
C	-4.164581	-1.606004	0.879353	C	4.970554	0.993511	-0.823669

C	-2.914231	-1.00452	0.916294	C	3.584536	0.985544	-0.753836
C	-2.598119	0.060802	0.062755	C	2.904443	0.012758	-0.009983
C	-3.585999	0.499741	-0.829057	C	3.667049	-0.950835	0.662226
C	-4.836573	-0.100614	-0.865108	C	5.053306	-0.941844	0.594006
C	-5.13293	-1.157456	-0.011604	C	5.712571	0.030114	-0.149708
H	-4.379892	-2.433457	1.542585	H	5.472142	1.749718	-1.413034
H	-2.162841	-1.381907	1.596521	H	3.021302	1.726375	-1.30488
H	-3.381031	1.337644	-1.481473	H	3.169427	-1.697201	1.26647
H	-5.585144	0.263862	-1.556306	H	5.620192	-1.691247	1.130462
H	-6.107423	-1.626006	-0.040637	H	6.792867	0.037092	-0.203279
C	-1.266489	0.698607	0.103226	C	1.428684	0.000613	0.064726
C	-0.657931	1.190355	-1.06552	C	0.712503	-1.206473	0.095454
C	-0.572151	0.855481	1.315681	C	0.688005	1.192027	0.081532
C	0.587469	1.782575	-1.034694	C	-0.663773	-1.226696	0.168318
H	-1.173613	1.094845	-2.01163	H	1.249293	-2.143298	0.031543
C	0.671755	1.449365	1.36006	C	-0.688806	1.183655	0.158398
H	-1.041447	0.542007	2.238484	H	1.205597	2.140835	0.040839
C	1.317007	1.860124	0.171731	C	-1.41232	-0.02887	0.278529
H	1.028854	2.156684	-1.948528	H	-1.182908	-2.174921	0.192494
H	1.170373	1.582658	2.310519	H	-1.23093	2.119103	0.14957
H	2.17271	2.516994	0.230897	H	-1.488022	-0.059132	2.079612
C	2.888659	0.259576	-0.074034	C	-2.89549	-0.02831	0.104889
C	2.547575	-0.904482	-0.723028	C	-3.701605	0.899896	0.770895
C	4.123783	0.484533	0.490422	C	-3.509471	-0.934219	-0.763072
C	3.513508	-1.908554	-0.813936	C	-5.074822	0.922481	0.574747
H	1.563587	-1.042693	-1.15338	H	-3.248639	1.591636	1.468534
C	5.082826	-0.526707	0.392332	C	-4.886022	-0.916127	-0.956567
H	4.359433	1.412391	0.998546	H	-2.904882	-1.644534	-1.310213
C	4.775076	-1.717249	-0.257876	C	-5.674421	0.012409	-0.289733
H	3.278702	-2.837238	-1.319287	H	-5.679976	1.644942	1.106314
H	6.065706	-0.380972	0.823266	H	-5.339503	-1.624775	-1.636944
H	5.520097	-2.498247	-0.331562	H	-6.745483	0.027595	-0.44039
tsp3i4 				tsp3i4(H)			
C	-0.414211	-0.549874	-1.065424	C	-0.70722	1.178563	-0.055701
C	-1.463814	-1.295858	-0.489532	C	0.701171	1.2163	0.002182
C	-1.501204	-2.677987	-0.708181	C	1.337418	2.462808	0.002468
C	-0.532184	-3.325704	-1.459249	C	0.620599	3.649155	-0.035806
C	0.509585	-2.592346	-2.010877	C	-0.766808	3.609984	-0.071602
C	0.559585	-1.221188	-1.81187	C	-1.415268	2.384684	-0.08207

H	-2.295429	-3.253172	-0.251347	H	2.417012	2.492754	0.06446
H	-0.586206	-4.396627	-1.602743	H	1.143007	4.596416	-0.026498
H	1.276365	-3.081334	-2.596508	H	-1.341881	4.525773	-0.098225
H	1.356908	-0.644566	-2.259977	H	-2.494756	2.350127	-0.136281
C	-0.317461	0.933419	-0.96417	C	-1.486284	-0.086971	-0.14331
C	-1.374383	1.758956	-1.373681	C	-1.229049	-1.050461	-1.131677
C	0.835583	1.569172	-0.517659	C	-2.5514	-0.361738	0.697376
C	-1.263914	3.142039	-1.327669	C	-2.004935	-2.197383	-1.235332
H	-2.286316	1.305625	-1.73855	H	-0.416942	-0.886442	-1.827202
C	0.9646	2.943052	-0.45116	C	-3.338466	-1.48798	0.636867
H	1.885054	0.871346	-0.075376	H	-2.855176	0.548889	1.836346
C	-0.097953	3.742438	-0.864935	C	-3.059063	-2.425669	-0.356586
H	-2.093571	3.753921	-1.655942	H	-1.785183	-2.91844	-2.011215
H	1.876726	3.390868	-0.077015	H	-4.147674	-1.644109	1.338814
H	-0.015921	4.820842	-0.824635	H	-3.65836	-3.322956	-0.440271
C	-2.519659	-0.697703	0.372941	C	1.550505	-0.00181	0.105542
C	-3.86984	-0.954819	0.115089	C	2.617443	-0.196252	-0.776979
C	-2.197543	0.084116	1.486463	C	1.343277	-0.949335	1.112489
C	-4.865828	-0.441665	0.937054	C	3.44518	-1.30673	-0.663962
H	-4.140398	-1.550677	-0.746803	H	2.789678	0.523003	-1.567053
C	-3.191198	0.592068	2.312064	C	2.173448	-2.055697	1.230111
H	-1.160292	0.289621	1.710954	H	0.53233	-0.811615	1.81408
C	-4.530165	0.333882	2.039912	C	3.22624	-2.241159	0.340766
H	-5.904439	-0.646659	0.712946	H	4.259967	-1.441662	-1.363128
H	-2.918194	1.189275	3.17204	H	1.999423	-2.773038	2.021215
H	-5.303879	0.732973	2.682064	H	3.870733	-3.105234	0.431656
C	2.996895	0.309122	0.40883	H	-3.0529	1.02467	2.514643
C	4.204136	0.636748	-0.17808				
C	2.905259	-0.552643	1.484858				
C	5.371783	0.074104	0.336931				
H	4.247985	1.313594	-1.022148				
C	4.077227	-1.111214	1.992962				
H	1.946813	-0.796512	1.924621				
C	5.305347	-0.796735	1.419465				
H	6.328888	0.316087	-0.107384				
H	4.029506	-1.790757	2.83433				
H	6.21254	-1.232121	1.816973				
tsi4i5				tsi5p4			
C	-0.975532	-1.094790	-0.055403	C	1.066432	-0.980431	-0.016832

C	-1.425398	0.244890	-0.108067	C	1.393668	0.396599	0.006004
C	-2.803532	0.476364	-0.184750	C	2.750683	0.762676	0.058046
C	-3.719246	-0.564571	-0.176605	C	3.758329	-0.177738	0.070275
C	-3.273566	-1.877117	-0.083347	C	3.436412	-1.535081	0.038292
C	-1.911128	-2.131112	-0.025939	C	2.114525	-1.920791	0.001049
H	-3.166703	1.491364	-0.262618	H	3.02339	1.805394	0.10692
H	-4.777405	-0.350214	-0.245001	H	4.791733	0.138523	0.115565
H	-3.979059	-2.696996	-0.072279	H	4.217302	-2.283288	0.058142
H	-1.554337	-3.151692	0.018720	H	1.888309	-2.975719	0.007664
C	0.469809	-1.408283	-0.024879	C	-0.330213	-1.397749	-0.030975
C	1.038042	-2.157426	0.998023	C	-0.704197	-2.739488	-0.193652
C	1.312360	-0.864707	-1.025326	C	-1.35814	-0.423727	0.193536
C	2.412336	-2.387275	1.038716	C	-2.024695	-3.138213	-0.186844
H	0.404015	-2.545098	1.784682	H	0.0547	-3.490101	-0.35176
C	2.690392	-1.143347	-1.002631	C	-2.71422	-0.861005	0.115338
H	0.868286	-0.494858	-1.938524	C	-3.038291	-2.183632	-0.039451
C	3.236435	-1.875800	0.037828	H	-2.273985	-4.18181	-0.321906
H	2.836856	-2.965717	1.848044	H	-3.510622	-0.141544	0.21794
H	3.320140	-0.781330	-1.804278	H	-4.076987	-2.484418	-0.065967
H	4.300511	-2.070642	0.062517	C	0.331125	1.404177	-0.027357
C	-0.473016	1.379435	-0.019938	C	0.619761	2.773259	-0.175016
C	-0.855585	2.646138	0.459386	C	-1.019542	1.011723	0.089736
C	0.861188	1.258143	-0.368848	C	-0.373355	3.729158	-0.178015
C	0.058522	3.688178	0.544266	H	1.641468	3.095522	-0.302646
H	-1.871405	2.811231	0.793116	C	-2.013666	2.00206	0.094269
C	1.799646	2.255595	-0.296549	C	-1.704251	3.340319	-0.03317
C	1.385361	3.505642	0.167011	H	-0.117717	4.773613	-0.295391
H	-0.266300	4.648937	0.920888	H	-3.051241	1.725533	0.196464
H	2.829864	2.083541	-0.583530	H	-2.493803	4.079595	-0.029534
H	2.093015	4.321732	0.240583	H	-1.234739	-0.434008	1.953116
Atom	X	Y	Z	Atom	X	Y	Z
tsi6				tsi6p5			
C	3.097598	-1.759147	0.820987	C	3.345068	-1.7996	0.150088
C	3.01473	-0.414955	1.083309	C	3.48482	-0.453611	-0.066314
C	2.123188	0.413019	0.360916	C	2.358446	0.403407	-0.085857
C	1.295043	-0.176219	-0.637626	C	1.058807	-0.15129	0.113173
C	1.407299	-1.558614	-0.887787	C	0.953092	-1.539378	0.352316
C	2.29008	-2.336273	-0.178018	C	2.06566	-2.344628	0.367311
H	2.683635	2.256765	1.337246	H	3.493597	2.201689	-0.44872

H	3.786046	-2.379712	1.37901	H	4.214601	-2.443041	0.163106
H	3.639199	0.033019	1.846163	H	4.465634	-0.022238	-0.222007
C	2.051291	1.813233	0.578792	C	2.500904	1.796663	-0.299409
C	0.368471	0.655227	-1.352495	C	-0.085089	0.734235	0.125333
H	0.778332	-2.005639	-1.647154	H	1.959049	-3.404669	0.555375
H	2.364806	-3.39588	-0.382642	C	0.117648	2.085636	-0.161349
C	0.406007	2.036959	-1.172416	C	1.401186	2.615878	-0.340193
C	1.220162	2.603277	-0.184196	H	-0.744193	2.734898	-0.231948
H	-0.108409	0.246095	-2.232029	H	1.517381	3.674682	-0.529286
H	-0.22972	2.670636	-1.775276	C	-1.487469	0.211814	0.064147
H	1.205132	3.67443	-0.031338	C	-2.473192	0.665536	0.943242
C	-1.652223	0.134839	-0.356425	C	-1.861437	-0.67886	-0.946969
C	-1.912662	0.650807	0.891594	C	-3.789702	0.238091	0.822057
C	-2.512653	-0.697622	-1.034757	H	-2.197316	1.347	1.736583
C	-3.117437	0.299266	1.503754	C	-3.177441	-1.106748	-1.069212
H	-1.21147	1.309151	1.388705	C	-4.147266	-0.651309	-0.183819
C	-3.716871	-1.039433	-0.413449	H	-4.53507	0.597402	1.51926
H	-2.278715	-1.085437	-2.019216	H	-3.445014	-1.792962	-1.861887
C	-4.013845	-0.542036	0.850973	H	-5.171612	-0.986299	-0.277411
H	-3.353598	0.684487	2.488024	H	-1.118711	-1.027022	-1.651816
H	-4.417557	-1.692188	-0.919386	H	-0.019804	-1.96859	0.540742
H	-4.946741	-0.809685	1.32897	H	-0.00276	0.934129	2.000741
tsi7				tsi7p6			
C	-3.967369	-1.025345	-0.56675	C	3.676245	0.965792	0.31989
C	-3.21879	-0.048162	-1.179388	C	2.740919	-1.575926	-0.36763
C	-2.087709	0.503721	-0.544332	C	4.085633	-1.349155	-0.226681
C	-1.721991	0.031402	0.755221	C	4.559427	-0.066938	0.119832
C	-2.518082	-0.972713	1.361133	H	4.038504	1.950408	0.58786
C	-3.612765	-1.489336	0.715844	H	2.376678	-2.559759	-0.635267
H	-1.604933	1.915487	-2.109639	H	4.790168	-2.15521	-0.382516
H	-4.832673	-1.439459	-1.066643	H	5.622752	0.09983	0.227705
H	-3.492927	0.312155	-2.163227	C	1.803074	-0.531195	-0.170684
C	-1.304701	1.533493	-1.14163	C	2.286378	0.76632	0.180197
C	-0.597726	0.590466	1.396532	C	0.415909	-0.73655	-0.30298
H	-2.244308	-1.330227	2.345829	C	1.339831	1.803862	0.396801
H	-4.208674	-2.257528	1.1905	C	-0.500637	0.310703	-0.183968
C	0.208108	1.530499	0.75473	H	0.06196	-1.72324	-0.571526
C	-0.211736	2.046045	-0.512224	C	0.005487	1.58904	0.239333
H	-0.340528	0.251845	2.391798	H	1.698286	2.778129	0.704999

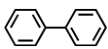


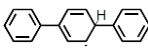
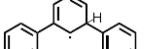


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H	0.368048	2.831782	-0.976959	C	-1.967699	0.043284	-0.090205
C	2.035344	0.335717	0.155187	C	-2.903557	0.959602	-0.579823
C	1.947897	-0.493709	-0.938902	C	-2.440275	-1.116551	0.528387
C	3.155663	0.437364	0.948297	C	-4.265137	0.722047	-0.459575
C	3.063474	-1.268669	-1.261354	H	-2.558422	1.852616	-1.083458
H	1.046883	-0.545475	-1.537212	C	-3.804191	-1.358306	0.645391
C	4.266792	-0.341424	0.614787	H	-1.736489	-1.825025	0.943061
H	3.190372	1.097157	1.807366	C	-4.722313	-0.440399	0.152424
C	4.21695	-1.190031	-0.486059	H	-4.97119	1.441229	-0.853237
H	3.029335	-1.931489	-2.117162	H	-4.147236	-2.261922	1.131715
H	5.165849	-0.282777	1.215803	H	-5.783855	-0.627002	0.244368
H	5.078749	-1.792486	-0.740543	H	-0.546659	0.728978	-1.944875
tsp5i8 				tsp5i9 			
C	4.166897	-1.615288	-1.308322	C	-2.347021	-3.162185	0.11971
C	3.605401	-2.219873	-0.215542	C	-3.394815	-2.288667	0.016594
C	2.52863	-1.618892	0.48103	C	-3.183292	-0.889341	-0.048179
C	2.033762	-0.350576	0.040834	C	-1.845047	-0.366789	0.023981
C	2.629014	0.235419	-1.105664	C	-0.803054	-1.320621	0.100032
C	3.665675	-0.377925	-1.76076	C	-1.025258	-2.666017	0.142546
H	2.310812	-3.213261	1.916852	H	-5.273888	-0.409102	-0.250045
H	4.987937	-2.087302	-1.831337	H	-2.522785	-4.229081	0.16457
H	3.975007	-3.176748	0.131308	H	-4.41213	-2.656526	-0.027476
C	1.926815	-2.254328	1.592592	C	-4.27285	0.000103	-0.197415
C	0.948236	0.252324	0.751714	C	-1.660831	1.051896	-0.01788
H	2.249554	1.178167	-1.471193	H	0.501809	-1.04891	0.033024
H	4.10011	0.088452	-2.635105	H	-0.190012	-3.353917	0.177113
C	0.388126	-0.417635	1.817125	C	-2.760577	1.86723	-0.1854
C	0.873108	-1.669606	2.240302	C	-4.064878	1.349253	-0.280379
H	-0.43364	0.038852	2.351791	H	-2.614603	2.938799	-0.212293
H	0.410053	-2.160331	3.085873	H	-4.899998	2.026328	-0.400728
C	0.415417	1.593063	0.3812	C	-0.3294	1.695096	0.14428
C	-0.90838	1.782401	0.00324	C	0.186926	2.519204	-0.859155
C	1.223074	2.738054	0.449771	C	0.395239	1.558389	1.331
C	-1.437194	3.02106	-0.304969	C	1.395082	3.183359	-0.683856
H	-1.738077	0.74185	-0.119602	H	-0.361771	2.632661	-1.785014
C	0.711839	3.995012	0.153199	C	1.597546	2.228908	1.510516
H	2.256284	2.636019	0.756128	H	0.004193	0.932952	2.122251
C	-0.617786	4.14431	-0.226493	C	2.103393	3.042038	0.503051

H	-2.472465	3.115169	-0.608089	H	1.782062	3.81134	-1.475595
H	1.35465	4.862492	0.22365	H	2.141256	2.114723	2.438823
H	-1.013376	5.124233	-0.460052	H	3.04295	3.559839	0.641771
C	-2.647922	-0.217992	-0.287682	C	1.833017	-1.139047	-0.108378
C	-3.740518	-0.244443	0.557465	C	2.566441	-1.680674	0.929494
C	-2.472508	-1.137193	-1.30402	C	2.409633	-0.748791	-1.300697
C	-4.700482	-1.239629	0.375919	C	3.943489	-1.829145	0.766768
H	-3.852776	0.48833	1.346737	H	2.088032	-1.980869	1.853236
C	-3.436886	-2.128931	-1.477888	C	3.787356	-0.899881	-1.45426
H	-1.605234	-1.094658	-1.950222	H	1.810495	-0.330641	-2.09878
C	-4.546217	-2.177676	-0.639509	C	4.549733	-1.438529	-0.422799
H	-5.565018	-1.280661	1.026279	H	4.538936	-2.24925	1.56747
H	-3.320147	-2.861581	-2.266284	H	4.262266	-0.597644	-2.379022
H	-5.292265	-2.948956	-0.777986	H	5.618198	-1.555438	-0.546757
tsp5i8 (H)				tsp5i9 (H)			
C	3.345771	-1.810361	0.277493	C	-3.338304	-1.805667	-0.165891
C	3.504362	-0.468652	0.05539	C	-3.492047	-0.455733	0.001158
C	2.384838	0.389923	-0.069285	C	-2.376048	0.416289	0.056128
C	1.067901	-0.162262	0.021102	C	-1.046706	-0.125456	-0.03974
C	0.944682	-1.552988	0.270437	C	-0.972361	-1.516908	-0.236355
C	2.050546	-2.353925	0.394214	C	-2.041023	-2.352182	-0.305713
H	3.547328	2.186668	-0.334218	H	-3.547661	2.213254	0.261136
H	4.210368	-2.45344	0.373668	H	-4.202135	-2.456171	-0.208439
H	4.495405	-0.039182	-0.021235	H	-4.482315	-0.026636	0.085931
C	2.545655	1.781685	-0.265336	C	-2.543769	1.814263	0.189236
C	-0.05677	0.712788	-0.107486	C	0.073007	0.760599	0.037031
H	-0.039775	-1.983622	0.377334	H	-1.907991	-3.412955	-0.476349
H	1.929126	-3.411091	0.58985	C	-0.156616	2.115564	0.146902
C	0.155993	2.063436	-0.277531	C	-1.458012	2.646166	0.219341
C	1.454164	2.60162	-0.357458	H	0.691106	2.78465	0.209348
H	-0.697231	2.721398	-0.371806	H	-1.591563	3.715379	0.315449
H	1.580143	3.6664	-0.50102	C	1.476186	0.268538	0.025247
C	-1.455828	0.206295	-0.074173	C	2.371629	0.705672	-0.95406
C	-2.387552	0.665714	0.840246	C	1.946962	-0.589746	1.022588
C	-1.930864	-0.727627	-1.0097	C	3.698284	0.291792	-0.941597
C	-3.704219	0.271605	0.894385	H	2.019848	1.364261	-1.73725
H	-1.961243	1.59885	1.924557	C	3.273835	-0.997357	1.040253
C	-3.255213	-1.147277	-0.995975	C	4.154282	-0.560137	0.056623
H	-1.252774	-1.108812	-1.762501	H	4.374309	0.634176	-1.713976

C	-4.147273	-0.654852	-0.048744	H	3.621394	-1.656291	1.82496
H	-4.375963	0.665132	1.646599	H	5.187216	-0.881378	0.068879
H	-3.594207	-1.861006	-1.734942	H	1.269352	-0.930448	1.793854
H	-5.177357	-0.986716	-0.041598	H	0.264749	-2.25271	-0.549508
H	-1.760979	2.114683	2.569835	H	0.887892	-2.789305	-0.780939
tsi8i10				tsi9i11			
C	2.699694	-2.145143	-0.201417	C	2.488954	2.305754	0.285994
C	3.169453	-0.851295	-0.285302	C	3.08668	1.068917	0.259232
C	2.301886	0.24955	-0.040479	C	2.314251	-0.107676	0.083082
C	0.955891	-0.019666	0.298484	C	0.910916	0.048287	-0.057792
C	0.525624	-1.368512	0.564406	C	0.343755	1.324955	-0.005378
C	1.403308	-2.417472	0.256868	C	1.081993	2.457112	0.133822
H	3.72223	1.829465	-0.429697	H	3.892801	-1.586866	0.146887
H	4.19596	-0.659191	-0.569205	H	3.096607	3.19135	0.425413
C	2.690104	1.600863	-0.196834	H	4.160066	0.983958	0.37162
C	-0.013862	1.007732	0.226151	C	2.826768	-1.427831	0.04329
H	1.11453	-3.438554	0.466452	C	0.046255	-1.06745	-0.226059
C	0.396542	2.319422	0.071617	H	0.640817	3.445588	0.147576
C	1.76057	2.611566	-0.095399	C	0.585206	-2.333996	-0.254582
H	-0.330277	3.117535	0.001276	C	1.981122	-2.500426	-0.123454
H	2.070202	3.640669	-0.22025	H	-0.047046	-3.201587	-0.39009
C	-2.669324	-1.544041	-0.315328	H	2.392678	-3.500681	-0.157114
C	-1.484298	-0.870681	-0.155093	C	-1.354082	-0.638419	-0.25196
C	-1.383209	0.491944	0.104967	C	-2.376136	-1.272975	0.43594
C	-2.576022	1.222479	0.159109	C	-1.562124	0.688673	-0.762809
C	-3.792872	0.581087	-0.043157	C	-3.591407	-0.626899	0.661831
C	-3.847191	-0.789199	-0.284984	H	-2.201707	-2.253605	0.859848
H	-2.703854	-2.612485	-0.48732	C	-2.800051	1.327812	-0.508978
H	-2.556132	2.284458	0.370307	C	-3.784906	0.683551	0.214261
H	-4.710045	1.153444	-0.00445	H	-4.373541	-1.130833	1.213029
H	-4.801436	-1.273142	-0.450717	H	-2.983066	2.311629	-0.92004
H	3.365465	-2.969749	-0.420885	H	-4.725746	1.182287	0.406674
H	-0.184403	-1.544254	1.362832	H	-1.035027	0.982425	-1.662448
tsi10p7				tsi11p7			
C	2.157908	-2.405857	-0.127171	C	2.166531	-2.417163	-0.05699
C	2.924582	-1.257255	-0.06137	C	2.932722	-1.271597	-0.072397
C	2.298423	0.016465	0.01317	C	2.309032	0.002511	-0.032378
C	0.90349	0.015373	0.074541	C	0.911033	0.003015	0.022344
C	0.106315	-1.165819	0.120844	C	0.122009	-1.165534	0.051293


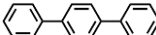

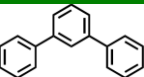


C	0.749204	-2.384877	-0.075469	C	0.750193	-2.385202	0.0087
H	3.999931	1.363775	-0.05782	H	4.013333	1.347482	-0.095205
H	4.003903	-1.325844	-0.104401	H	4.011888	-1.343093	-0.118595
C	2.920642	1.290298	-0.019994	C	2.934003	1.27631	-0.052687
C	0.105861	1.174836	0.039374	C	0.117456	1.173049	0.045304
H	0.195833	-3.312218	-0.137969	H	0.197322	-3.315157	0.032102
C	0.735903	2.399473	-0.003762	C	0.753407	2.394029	0.026349
C	2.1506	2.435591	-0.020289	C	2.168722	2.423505	-0.021089
H	0.179132	3.326811	-0.037888	H	0.202154	3.325127	0.044544
H	2.642602	3.398858	-0.051172	H	2.664404	3.385284	-0.036215
C	-2.49614	-1.397137	0.001694	C	-2.495303	-1.398618	-0.058645
C	-1.300598	-0.700261	0.041786	C	-1.288044	-0.707818	0.134969
C	-1.293169	0.718501	0.016179	C	-1.278159	0.728187	0.064183
C	-2.488558	1.419598	-0.040351	C	-2.470635	1.42637	-0.012792
C	-3.687406	0.710125	-0.079879	C	-3.669643	0.719278	-0.094827
C	-3.691338	-0.682128	-0.062646	C	-3.675893	-0.677573	-0.141422
H	-2.509874	-2.479022	0.024139	H	-2.508302	-2.479595	-0.096757
H	-2.496293	2.501679	-0.059051	H	-2.476929	2.508346	-0.039176
H	-4.625596	1.246657	-0.12674	H	-4.605036	1.258526	-0.158798
H	-4.632232	-1.214786	-0.09705	H	-4.615668	-1.201793	-0.251967
H	2.655527	-3.361402	-0.228261	H	2.659539	-3.379747	-0.091936
H	0.012759	-1.266063	1.976263	H	-1.2673	-0.841882	1.95253

Table S6. Harmonic Frequencies (cm^{-1}) of relevant reactants, intermediates, transition states and products.

							
v1	65.4	413.9	403.0	16.3	22.1	23.5	36.9
v2	95.2	413.9	429.2	23.7	35.0	38.0	49.8
v3	128.0	624.2	602.3	46.0	45.3	49.0	62.1
v4	268.5	624.2	621.3	96.1	81.8	76.9	88.8
v5	314.5	689.7	678.6	103.6	116.5	111.7	103.5
v6	371.8	726.6	725.6	141.0	118.4	147.3	137.1
v7	416.5	866.6	818.1	214.9	214.1	191.8	226.0
v8	422.5	866.6	899.4	234.6	239.4	251.4	256.9
v9	503.3	987.8	972.2	275.4	282.1	262.7	276.5
v10	561.6	987.8	994.6	305.4	307.8	308.0	320.1
v11	627.4	1015.4	1001.7	392.9	340.8	346.6	365.3
v12	630.2	1021.1	1018.9	407.8	366.2	415.2	402.1
v13	642.6	1030.7	1052.5	416.7	417.0	416.9	417.5
v14	716.6	1062.3	1074.6	417.8	419.4	423.2	428.2
v15	720.7	1062.3	1177.9	420.3	448.4	461.0	508.2
v16	758.3	1176.8	1178.2	492.8	515.6	510.6	534.8
v17	760.4	1200.6	1305.7	546.7	551.9	524.5	567.8
v18	803.6	1200.6	1327.6	548.5	597.2	568.5	576.8
v19	862.6	1335.0	1468.3	602.4	610.2	595.2	619.1
v20	862.7	1390.2	1476.1	606.9	613.0	610.0	629.0
v21	931.9	1518.9	1575.0	636.9	635.7	635.4	637.0
v22	950.7	1518.9	1630.2	637.2	638.5	638.5	640.6
v23	991.3	1637.5	3157.3	683.7	649.3	677.0	712.3
v24	992.1	1637.5	3163.1	705.8	708.2	699.8	717.9
v25	1008.3	3157.7	3176.1	717.9	718.0	706.9	724.3
v26	1008.4	3167.4	3178.3	730.1	719.6	718.0	750.1
v27	1014.9	3167.4	3189.5	751.0	754.5	750.2	767.9
v28	1023.3	3183.1		752.6	773.6	775.3	785.9
v29	1031.8	3183.1		784.6	783.4	784.0	787.7
v30	1056.4	3193.2		793.4	801.0	791.9	799.3
v31	1069.3			849.2	818.9	845.2	861.8
v32	1104.8			857.2	861.4	850.5	862.6
v33	1109.3			861.8	863.2	859.7	901.2
v34	1184.6			915.3	864.1	923.4	939.6



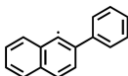




v35	1185.4	925.4	913.9	930.2	951.8
v36	1206.3	934.4	934.4	939.7	977.3
v37	1213.8	980.2	942.6	946.4	989.3
v38	1298.8	982.9	978.5	978.5	991.2
v39	1303.9	984.4	987.0	984.4	993.3
v40	1326.5	987.3	991.5	986.4	1002.5
v41	1363.3	987.8	1003.5	1000.7	1006.5
v42	1365.0	1001.6	1007.6	1001.6	1018.0
v43	1467.2	1006.3	1007.8	1005.6	1026.1
v44	1495.5	1008.3	1016.6	1016.6	1031.4
v45	1522.7	1022.2	1023.6	1021.8	1056.6
v46	1543.2	1024.0	1026.0	1023.6	1060.9
v47	1611.3	1044.3	1053.7	1036.0	1088.0
v48	1626.2	1053.6	1058.0	1053.7	1104.9
v49	1643.3	1056.5	1061.6	1057.7	1118.8
v50	1646.5	1104.0	1103.5	1103.7	1143.9
v51	3161.6	1108.7	1103.9	1111.5	1177.8
v52	3162.5	1170.7	1128.3	1144.0	1184.2
v53	3167.3	1183.6	1183.2	1183.0	1190.0
v54	3170.0	1184.0	1184.3	1185.1	1207.4
v55	3177.4	1194.6	1185.1	1187.2	1240.8
v56	3181.2	1206.1	1199.5	1195.7	1276.6
v57	3183.2	1208.4	1205.8	1205.8	1283.4
v58	3186.4	1215.9	1207.8	1215.0	1302.6
v59	3192.0	1238.1	1225.8	1227.7	1319.6
v60	3193.4	1260.4	1272.1	1266.3	1322.4
v61		1311.8	1290.5	1284.1	1328.0
v62		1313.2	1298.2	1309.9	1360.5
v63		1328.0	1334.9	1333.2	1440.0
v64		1338.1	1339.6	1341.1	1469.4
v65		1363.5	1345.6	1365.6	1480.7
v66		1367.8	1365.2	1368.2	1488.8
v67		1416.6	1367.1	1408.0	1516.3
v68		1470.6	1441.9	1427.9	1536.6
v69		1478.3	1482.6	1480.9	1569.7
v70		1488.9	1488.3	1488.0	1604.1
v71		1526.0	1528.0	1523.6	1619.6
v72		1529.6	1529.7	1529.1	1634.2
v73		1531.6	1560.7	1534.5	1638.0

v74	1604.1	1589.2	1606.6	1644.6
v75	1604.6	1619.7	1609.7	3157.8
v76	1626.0	1627.1	1626.5	3161.0
v77	1637.3	1642.8	1635.4	3164.0
v78	1644.1	1644.3	1642.1	3165.3
v79	2910.5	2887.6	2938.3	3168.2
v80	3154.0	3153.8	3149.8	3174.3
v81	3159.3	3155.7	3158.3	3175.8
v82	3159.8	3161.5	3162.6	3177.8
v83	3162.2	3162.6	3162.8	3183.8
v84	3164.0	3167.7	3169.0	3184.3
v85	3167.2	3171.3	3172.1	3187.9
v86	3170.0	3172.0	3172.3	3191.8
v87	3179.2	3177.9	3178.0	3192.9
v88	3179.5	3178.9	3180.7	
v89	3180.4	3179.9	3186.7	
v90	3186.7	3184.3	3190.2	
v91	3188.9	3190.1	3193.3	
v92	3193.2	3192.1	3196.8	
v93	3200.4	3198.5	3200.8	

						
v1	65.4	37.9	37.5	46.6	52.2	51.3
v2	75.2	45.5	44.6	47.9	54.0	51.3
v3	107.7	68.5	69.7	62.7	62.3	110.8
v4	132.9	81.6	79.9	96.5	93.6	121.7
v5	206.0	122.9	111.8	114.8	103.9	261.1
v6	226.9	137.1	153.0	143.2	134.9	261.1
v7	267.6	214.6	215.3	236.7	234.2	274.2
v8	311.1	245.5	225.8	274.2	255.5	274.2
v9	360.1	295.0	338.4	284.8	275.2	410.6
v10	380.4	393.1	344.7	333.5	324.3	410.6
v11	398.6	408.4	407.8	350.8	364.1	422.2
v12	430.9	416.8	416.4	406.9	399.9	434.4
v13	453.4	419.8	418.9	421.1	417.8	438.9
v14	457.1	424.4	428.0	421.1	419.1	438.9
v15	514.6	425.1	460.7	492.0	520.0	556.5
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v17	568.3	534.1	545.2	551.6	572.9	567.7

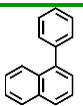
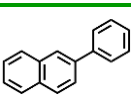
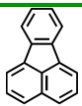
v18	578.9	584.0	584.4	628.5	577.3	586.1
v19	596.8	629.1	629.0	629.7	629.9	621.2
v20	614.6	633.4	632.6	632.9	632.3	637.4
v21	635.9	636.1	637.0	637.3	639.1	637.4
v22	683.8	658.7	658.4	649.1	641.3	713.8
v23	699.0	714.6	714.6	718.3	719.8	729.4
v24	723.3	718.6	718.1	719.5	720.0	729.4
v25	750.3	718.9	718.4	725.9	725.4	758.9
v26	763.8	750.9	752.9	727.2	766.3	790.0
v27	771.9	777.3	774.2	774.4	767.4	790.0
v28	783.2	792.3	792.1	788.9	789.0	791.3
v29	791.9	796.3	798.6	824.6	795.2	791.3
v30	798.2	857.0	857.1	828.5	804.1	794.2
v31	847.4	862.8	862.2	864.0	862.9	871.3
v32	886.4	862.8	862.3	864.5	862.9	871.3
v33	903.5	869.5	869.7	927.7	900.0	890.4
v34	943.2	938.8	940.1	929.7	940.2	949.9
v35	946.9	944.7	942.7	947.7	943.9	949.9
v36	964.9	987.0	987.1	952.0	977.1	968.5
v37	970.7	991.4	991.1	993.2	990.8	984.6
v38	984.4	991.4	991.3	993.2	991.1	994.6
v39	994.1	995.0	993.9	1000.5	1002.6	994.6
v40	996.0	1007.7	1007.6	1009.3	1007.7	1022.2
v41	1004.4	1007.9	1007.8	1009.3	1008.1	1022.2
v42	1017.9	1016.1	1016.0	1013.5	1017.1	1028.7
v43	1025.9	1020.1	1020.6	1021.3	1019.8	1079.5
v44	1044.9	1028.3	1028.1	1022.5	1029.6	1079.5
v45	1076.7	1030.5	1030.3	1034.0	1031.3	1089.5
v46	1080.0	1050.0	1050.0	1052.4	1059.9	1137.1
v47	1118.3	1061.9	1062.0	1065.5	1061.2	1137.1
v48	1137.4	1071.9	1071.9	1087.1	1086.9	1172.9
v49	1154.5	1106.4	1106.3	1106.1	1103.9	1195.3
v50	1186.0	1106.9	1106.9	1106.6	1106.2	1195.3
v51	1189.4	1144.7	1145.1	1122.4	1141.6	1208.3
v52	1196.4	1184.7	1184.8	1184.9	1184.1	1247.1
v53	1203.6	1184.8	1185.0	1184.9	1184.5	1273.2
v54	1229.9	1207.2	1207.3	1200.0	1189.3	1273.2
v55	1253.8	1209.3	1209.3	1208.8	1207.4	1321.3
v56	1267.2	1220.5	1220.7	1209.3	1208.5	1321.3

v57	1295.9	1287.1	1287.0	1265.0	1267.4	1325.4
v58	1304.9	1304.3	1304.1	1291.7	1277.7	1359.8
v59	1315.8	1307.6	1307.2	1308.7	1302.9	1368.3
v60	1331.4	1310.2	1309.7	1324.1	1311.1	1368.3
v61	1335.7	1323.7	1324.1	1331.8	1322.6	1472.5
v62	1344.4	1349.0	1349.1	1352.9	1327.4	1472.5
v63	1406.1	1360.7	1360.8	1358.6	1360.3	1480.4
v64	1435.7	1365.5	1365.5	1365.2	1361.2	1496.7
v65	1473.5	1436.2	1436.3	1437.3	1466.1	1537.0
v66	1486.1	1477.8	1477.8	1480.1	1478.8	1537.0
v67	1509.2	1489.5	1489.5	1492.5	1489.6	1589.7
v68	1522.4	1523.4	1523.5	1516.3	1512.5	1618.8
v69	1533.2	1533.1	1533.2	1534.8	1533.4	1618.8
v70	1594.3	1557.2	1557.0	1539.4	1539.1	1648.0
v71	1610.1	1588.5	1588.2	1610.4	1601.6	1648.0
v72	1619.1	1618.7	1618.8	1617.6	1618.0	1654.1
v73	1633.1	1623.0	1623.2	1626.2	1622.7	3167.3
v74	1642.0	1642.5	1642.3	1640.1	1638.0	3168.4
v75	2825.8	1644.5	1644.4	1645.2	1644.9	3168.4
v76	3159.0	1652.4	1652.3	1645.3	1645.0	3182.2
v77	3163.7	3162.1	3162.2	3162.0	3160.4	3182.2
v78	3165.9	3162.3	3162.4	3162.0	3160.5	3184.9
v79	3167.3	3167.1	3167.3	3165.9	3163.9	3199.0
v80	3176.5	3168.6	3168.9	3168.5	3167.8	3202.0
v81	3179.9	3169.0	3169.1	3168.7	3168.0	3202.0
v82	3182.9	3171.3	3171.6	3177.6	3172.6	3219.8
v83	3187.7	3179.1	3179.2	3178.2	3177.3	3219.8
v84	3192.6	3180.1	3180.3	3181.1	3177.5	3221.9
v85	3196.1	3183.1	3183.3	3182.3	3182.1	
v86	3198.1	3185.4	3185.6	3185.2	3185.7	
v87	3201.3	3187.1	3187.4	3185.8	3185.7	
v88		3187.6	3188.0	3191.1	3191.8	
v89		3192.8	3193.0	3192.6	3192.9	
v90		3193.2	3193.4	3193.2	3193.0	

							
v1	173.2	29.0	23.0	46.0	52.3	95.7	89.7
v2	187.1	36.3	35.0	71.2	74.9	114.9	97.8

v3	366.4	66.0	77.5	91.0	88.3	158.9	170.5
v4	397.7	155.4	163.3	170.9	169.8	197.6	191.1
v5	482.9	172.8	179.0	181.3	183.0	231.6	240.6
v6	489.3	244.2	251.4	248.5	241.8	282.6	269.5
v7	519.8	264.7	274.7	293.3	293.6	341.8	348.4
v8	521.1	299.7	292.2	315.5	317.2	411.1	411.3
v9	637.3	380.5	372.3	411.9	414.7	436.4	424.1
v10	639.4	416.4	406.3	427.0	419.4	467.3	465.1
v11	732.5	430.5	416.8	446.3	456.3	477.5	481.3
v12	775.3	479.5	458.1	484.2	476.4	492.5	490.9
v13	792.5	483.9	506.6	503.6	503.0	536.9	521.4
v14	803.3	515.3	529.5	531.0	526.2	548.8	560.5
v15	811.6	537.1	539.6	562.7	565.9	558.0	566.0
v16	853.4	562.9	558.5	583.9	584.5	608.0	592.6
v17	904.8	617.2	617.4	623.8	630.3	617.5	625.9
v18	956.6	634.4	635.5	632.5	633.6	633.3	637.9
v19	964.8	650.1	644.9	663.1	650.5	676.4	647.3
v20	982.0	690.0	713.1	706.9	712.4	694.8	688.0
v21	997.4	719.3	716.5	719.3	717.5	745.5	738.3
v22	1003.4	728.8	723.2	749.1	752.6	760.6	762.3
v23	1037.3	760.1	754.2	757.8	776.4	762.8	776.9
v24	1047.8	774.9	766.2	800.3	786.2	781.9	791.9
v25	1154.6	795.6	779.3	809.2	802.6	800.1	812.2
v26	1170.9	799.6	798.8	822.0	834.2	822.5	817.7
v27	1174.6	811.2	824.0	844.2	846.1	847.4	850.7
v28	1187.4	845.7	854.1	863.1	860.6	879.3	879.8
v29	1234.6	861.3	861.6	890.2	892.1	892.7	899.0
v30	1275.4	891.1	874.7	933.8	929.4	899.8	916.3
v31	1292.1	931.4	907.8	953.7	943.5	957.8	924.8
v32	1393.1	939.8	933.4	976.6	965.0	962.9	970.3
v33	1397.4	965.9	950.0	980.0	979.4	971.8	976.0
v34	1424.9	971.4	956.2	992.1	990.5	978.7	980.3
v35	1496.2	987.0	981.7	994.7	993.5	995.1	986.8
v36	1496.9	991.9	987.4	996.6	1007.5	1026.3	991.4
v37	1551.3	999.3	1001.4	1002.7	1020.5	1047.4	1026.0
v38	1614.2	1007.8	1007.5	1046.1	1042.9	1070.2	1055.0
v39	1642.7	1023.3	1023.3	1051.2	1054.8	1075.3	1066.1
v40	1670.3	1053.6	1043.7	1086.2	1087.1	1108.2	1074.3
v41	3156.7	1062.3	1053.5	1123.0	1107.2	1133.5	1130.2

v42	3158.6	1097.1	1084.0	1143.3	1134.9	1159.1	1150.5
v43	3160.8	1103.6	1103.5	1171.9	1168.2	1175.1	1164.5
v44	3164.2	1142.0	1140.8	1178.2	1184.8	1182.2	1181.2
v45	3175.0	1178.9	1165.3	1189.0	1191.8	1194.3	1195.8
v46	3176.3	1182.3	1178.5	1211.2	1208.5	1198.9	1209.9
v47	3187.9	1183.6	1183.7	1233.5	1212.5	1228.0	1236.5
v48	3188.9	1194.7	1196.4	1252.4	1240.8	1234.3	1255.5
v49		1205.5	1205.7	1275.3	1304.2	1286.3	1274.8
v50		1207.3	1208.6	1308.3	1312.8	1293.8	1289.7
v51		1234.0	1229.0	1324.3	1348.5	1320.0	1323.5
v52		1237.8	1257.6	1363.5	1354.3	1324.8	1364.6
v53		1275.1	1300.3	1386.3	1366.4	1360.6	1383.7
v54		1306.0	1317.7	1429.6	1401.5	1380.9	1399.0
v55		1338.3	1339.0	1440.8	1459.9	1426.7	1424.5
v56		1340.8	1342.5	1476.6	1462.6	1469.8	1437.7
v57		1369.0	1367.5	1479.9	1485.8	1473.8	1463.9
v58		1391.6	1416.5	1499.6	1513.6	1496.4	1484.9
v59		1441.6	1432.7	1548.5	1532.6	1508.0	1523.1
v60		1472.2	1463.4	1568.3	1589.5	1530.4	1525.1
v61		1488.6	1488.3	1614.0	1615.2	1610.3	1597.3
v62		1518.3	1506.0	1629.6	1634.2	1617.5	1613.4
v63		1529.9	1529.6	1637.3	1642.4	1620.4	1627.9
v64		1555.3	1562.6	1661.5	1653.1	1647.5	1648.4
v65		1596.7	1604.0	3158.8	3158.1	2841.5	2827.6
v66		1626.3	1626.0	3159.2	3161.3	3155.9	3156.8
v67		1628.4	1641.9	3162.4	3161.7	3160.5	3159.9
v68		1642.8	1669.5	3165.5	3168.9	3161.7	3160.4
v69		2943.0	2906.2	3170.7	3169.4	3167.0	3161.3
v70		3153.1	3146.7	3174.7	3174.9	3174.1	3170.7
v71		3154.7	3153.4	3176.0	3179.7	3177.8	3174.9
v72		3157.2	3156.3	3185.2	3181.7	3178.7	3178.8
v73		3162.0	3159.7	3187.7	3186.9	3185.9	3183.6
v74		3162.4	3162.0	3188.9	3188.8	3187.1	3185.8
v75		3171.2	3162.7	3199.6	3193.4	3190.1	3191.7
v76		3174.5	3171.0				
v77		3175.6	3171.1				
v78		3179.2	3175.6				
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v80		3189.1	3189.3				


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v2	75.4	62.8	122.9
v3	84.8	94.2	166.8
v4	169.4	172.8	207.6
v5	183.7	188.5	257.2
v6	245.2	262.9	299.3
v7	293.6	278.3	357.1
v8	316.5	339.6	440.1
v9	411.7	404.6	441.7
v10	418.4	419.7	471.0
v11	446.7	437.2	478.5
v12	483.9	490.1	494.6
v13	505.5	516.7	571.8
v14	531.9	529.0	572.8
v15	571.8	560.6	579.9
v16	587.4	571.2	629.0
v17	633.9	634.3	637.9
v18	635.5	644.5	656.9
v19	670.7	674.0	686.8
v20	712.3	711.9	755.8
v21	722.0	718.0	762.0
v22	752.5	758.9	779.2
v23	783.9	780.5	796.7
v24	801.9	787.3	803.1
v25	809.8	796.5	820.0
v26	825.7	841.2	850.6
v27	845.3	862.4	891.2
v28	865.8	872.4	909.3
v29	891.8	882.1	922.4
v30	931.9	925.0	931.0
v31	945.5	944.9	957.4
v32	978.5	962.6	982.9
v33	983.4	973.4	991.1
v34	992.0	990.0	992.1
v35	993.6	992.2	995.1

v36	1004.0	1000.1	1040.9
v37	1009.8	1008.3	1045.9
v38	1021.3	1020.2	1063.5
v39	1046.8	1039.9	1109.6
v40	1054.9	1046.4	1125.4
v41	1083.7	1065.6	1164.2
v42	1104.3	1107.0	1185.1
v43	1142.8	1157.8	1187.2
v44	1171.7	1175.5	1210.7
v45	1184.3	1184.1	1237.3
v46	1187.8	1185.5	1258.5
v47	1207.0	1209.1	1294.9
v48	1210.8	1221.2	1322.7
v49	1237.5	1258.9	1342.3
v50	1275.9	1294.2	1398.0
v51	1309.5	1301.5	1405.4
v52	1316.7	1316.5	1444.9
v53	1354.9	1357.5	1458.0
v54	1369.5	1384.0	1476.5
v55	1386.9	1398.1	1490.1
v56	1430.1	1405.8	1510.0
v57	1468.8	1464.7	1525.7
v58	1484.0	1488.5	1616.1
v59	1497.6	1504.5	1641.7
v60	1531.7	1534.2	1643.7
v61	1548.9	1546.4	1646.2
v62	1613.9	1605.7	1659.0
v63	1618.5	1619.5	3161.7
v64	1636.6	1643.7	3162.4
v65	1643.7	1644.5	3162.4
v66	1661.2	1668.6	3168.3
v67	3158.7	3157.7	3172.1
v68	3160.9	3160.4	3173.0
v69	3161.4	3161.3	3178.6
v70	3167.5	3163.1	3185.2
v71	3170.2	3166.5	3186.0
v72	3172.5	3169.4	3190.6
v73	3177.3	3175.9	
v74	3183.0	3178.1	

v75 3185.2 3183.2
v76 3186.7 3185.7
v77 3191.2 3188.6
v78 3202.6 3192.0

	tsi1	tsi1p1	tsi2	tsi2p2	tsi3	tsi3p3	tsp3i4 (H)
v1	-317.1	-917.5	-332.0	-949.3	-320.7	-819.2	-898.2
v2	15.0	37.4	14.5	42.8	25.8	47.9	44.9
v3	26.0	46.1	27.3	46.1	37.0	54.1	49.1
v4	43.5	66.4	46.1	59.1	49.1	60.3	58.7
v5	76.0	83.7	80.3	97.4	78.0	102.3	90.4
v6	93.0	126.5	94.3	113.2	96.8	107.5	101.5
v7	116.8	137.0	108.5	143.8	122.6	138.6	128.0
v8	138.5	213.6	144.2	233.3	139.9	225.8	182.3
v9	164.3	240.2	171.6	268.9	165.6	255.7	233.2
v10	262.3	294.0	271.3	269.5	243.4	281.9	246.2
v11	320.6	383.2	314.6	328.0	322.3	314.3	260.0
v12	368.5	403.2	358.1	350.6	361.3	358.6	290.6
v13	400.8	406.0	390.2	404.3	394.4	406.7	322.6
v14	417.0	418.9	399.9	419.2	400.4	418.5	362.2
v15	422.6	419.5	421.0	419.2	421.5	419.4	400.2
v16	443.2	421.6	445.8	439.7	447.9	453.7	418.5
v17	467.5	447.3	499.5	488.3	498.9	508.0	424.4
v18	534.1	522.0	545.0	505.1	562.1	534.3	520.2
v19	582.8	527.5	590.9	552.5	577.6	558.7	531.1
v20	614.9	557.5	615.4	564.6	614.9	570.9	573.6
v21	623.1	585.6	624.3	628.2	623.0	577.8	576.4
v22	625.7	631.5	626.0	631.6	624.1	628.7	620.2
v23	640.3	633.6	638.7	637.4	639.7	632.5	624.3
v24	696.0	636.6	691.3	639.8	696.0	638.3	634.5
v25	715.9	653.9	696.6	648.5	715.7	640.8	638.8
v26	718.1	711.8	719.1	704.9	718.6	713.8	714.9
v27	730.8	716.8	731.4	718.1	732.5	718.5	720.2
v28	753.2	718.5	756.9	718.5	750.4	719.5	725.8
v29	772.7	745.3	767.9	727.3	754.5	759.6	759.5
v30	813.4	776.9	802.0	773.0	796.4	772.2	767.3
v31	839.3	786.1	839.6	787.4	839.9	786.7	787.1
v32	842.1	798.5	863.8	818.5	861.4	792.9	788.1
v33	860.8	843.6	866.0	829.4	864.3	805.9	801.3



v34	885.3	860.5	905.4	861.0	894.2	860.5	863.8
v35	907.4	861.1	906.1	863.4	907.9	863.0	869.9
v36	937.9	867.2	907.0	911.6	939.3	896.1	900.5
v37	972.2	938.5	945.1	925.0	966.4	939.4	927.9
v38	975.2	943.0	971.7	943.9	972.9	943.9	942.2
v39	988.9	987.6	989.3	946.5	991.2	974.5	959.9
v40	991.3	990.0	992.0	990.4	992.8	989.5	972.1
v41	997.6	991.7	997.3	992.4	999.1	992.0	978.7
v42	999.8	993.3	1000.0	997.0	1000.5	999.7	991.7
v43	1007.0	1007.9	1008.4	1004.9	1007.8	1007.5	998.8
v44	1012.1	1008.3	1010.1	1008.5	1009.8	1008.6	1004.1
v45	1020.6	1012.4	1020.3	1009.3	1020.7	1014.0	1008.6
v46	1022.8	1020.3	1024.3	1020.7	1024.8	1020.1	1018.1
v47	1031.4	1023.1	1038.5	1021.9	1036.2	1025.6	1023.6
v48	1043.6	1027.5	1050.0	1032.8	1054.2	1029.7	1028.9
v49	1058.6	1043.4	1062.4	1051.2	1058.2	1058.7	1031.4
v50	1064.6	1060.9	1065.3	1064.8	1064.7	1060.7	1059.9
v51	1081.8	1067.3	1082.7	1077.9	1082.3	1081.0	1063.8
v52	1093.4	1106.1	1089.1	1105.7	1088.6	1103.7	1087.1
v53	1107.3	1107.6	1106.8	1106.6	1110.4	1106.5	1103.9
v54	1178.6	1144.7	1178.4	1120.4	1179.0	1140.7	1130.9
v55	1178.7	1184.9	1178.8	1184.7	1182.4	1184.0	1143.3
v56	1184.9	1185.4	1184.6	1185.0	1185.7	1184.8	1182.0
v57	1185.8	1207.3	1186.3	1197.0	1185.9	1188.1	1184.4
v58	1205.3	1209.6	1193.9	1208.8	1200.0	1207.9	1189.8
v59	1212.1	1216.3	1209.2	1209.3	1215.1	1209.8	1208.3
v60	1287.5	1274.6	1294.1	1256.2	1291.4	1259.2	1252.2
v61	1305.3	1290.7	1296.9	1282.5	1292.3	1267.8	1267.2
v62	1321.2	1305.6	1321.7	1308.8	1320.8	1296.5	1286.4
v63	1322.9	1307.7	1322.6	1321.7	1322.5	1305.3	1307.8
v64	1329.2	1322.5	1329.8	1322.3	1328.8	1321.4	1316.9
v65	1362.3	1344.2	1355.6	1348.9	1359.0	1328.2	1322.4
v66	1365.0	1361.1	1362.3	1358.1	1367.1	1360.1	1327.0
v67	1468.0	1365.0	1451.1	1363.5	1449.7	1363.3	1361.8
v68	1469.7	1441.9	1469.8	1420.0	1469.6	1459.7	1446.6
v69	1484.5	1476.3	1484.7	1479.5	1484.5	1475.1	1469.3
v70	1494.2	1489.4	1489.0	1489.1	1490.0	1487.2	1485.0
v71	1506.4	1516.1	1511.6	1506.8	1516.4	1499.8	1486.3
v72	1536.1	1532.8	1535.6	1533.3	1538.3	1531.4	1517.9

v73	1563.8	1543.8	1580.0	1535.4	1575.8	1533.7	1536.5
v74	1583.1	1557.6	1586.4	1592.7	1583.9	1579.3	1580.0
v75	1611.8	1618.2	1602.8	1611.6	1610.0	1615.1	1603.6
v76	1616.9	1621.3	1620.7	1621.8	1618.1	1619.6	1619.6
v77	1627.7	1629.3	1627.7	1624.4	1626.9	1624.6	1628.8
v78	1642.5	1643.9	1644.6	1644.2	1642.2	1642.6	1639.0
v79	3144.2	1645.0	3143.8	1645.0	3144.0	1643.2	1644.1
v80	3153.8	3161.8	3154.7	3161.7	3155.0	3160.7	2315.3
v81	3162.1	3162.1	3161.4	3161.8	3162.4	3161.0	3159.7
v82	3162.8	3167.8	3162.3	3167.0	3164.0	3166.3	3160.5
v83	3165.6	3169.0	3163.7	3168.3	3165.5	3168.6	3164.7
v84	3167.8	3171.3	3166.6	3168.9	3170.0	3168.6	3168.0
v85	3169.5	3173.3	3168.9	3177.6	3171.4	3175.7	3169.8
v86	3171.5	3178.4	3171.2	3177.8	3172.7	3177.7	3174.5
v87	3177.0	3180.0	3178.0	3182.8	3178.0	3178.3	3177.5
v88	3181.5	3184.0	3182.5	3183.5	3183.5	3185.7	3178.0
v89	3184.5	3185.2	3183.7	3186.5	3185.8	3186.3	3183.9
v90	3185.0	3189.5	3185.0	3187.6	3186.7	3186.7	3185.7
v91	3187.8	3190.7	3186.3	3191.7	3191.6	3193.0	3189.6
v92	3191.9	3192.4	3191.7	3192.1	3194.9	3193.4	3192.6
v93	3193.6	3193.4	3193.1	3194.3	3200.8	3194.2	3193.0
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	tsp3i4 	tsi4i5	tsi5p4				
v1	-1623.1	-249.3	-959.6				
v2	12.5	56.2	52.1				
v3	15.4	76.0	62.6				
v4	25.9	98.6	113.7				
v5	48.3	106.7	122.2				
v6	51.3	164.4	247.9				
v7	60.9	222.2	250.1				
v8	87.5	238.4	272.7				
v9	98.0	271.0	286.3				
v10	112.2	335.1	386.2				
v11	142.2	372.5	407.0				
v12	154.7	399.5	408.2				
v13	177.2	411.7	426.8				
v14	240.8	442.1	437.0				
v15	262.1	471.3	442.8				
v16	288.3	546.5	487.8				

v17	326.9	563.1	502.0
v18	366.5	581.7	560.0
v19	400.6	589.6	562.5
v20	404.9	620.4	575.3
v21	418.5	627.4	584.3
v22	430.3	632.7	623.2
v23	442.0	712.3	634.9
v24	522.7	721.4	638.3
v25	535.9	734.3	708.0
v26	574.7	749.1	730.2
v27	577.9	756.0	738.8
v28	619.6	782.6	757.8
v29	620.8	787.3	784.9
v30	627.2	797.6	790.1
v31	634.2	851.5	791.6
v32	639.6	869.6	796.1
v33	680.1	891.0	802.8
v34	702.3	898.5	876.4
v35	719.4	951.1	877.6
v36	727.1	959.5	898.9
v37	729.3	974.1	959.0
v38	737.3	990.7	961.5
v39	763.8	991.9	969.3
v40	766.8	999.0	989.0
v41	789.8	1001.4	995.5
v42	790.4	1014.7	996.6
v43	802.1	1025.4	1015.0
v44	849.3	1034.8	1022.8
v45	863.1	1055.0	1027.9
v46	881.0	1061.3	1072.2
v47	900.4	1082.5	1079.8
v48	914.4	1089.1	1086.5
v49	941.2	1122.7	1133.8
v50	963.2	1144.4	1134.8
v51	977.9	1181.4	1171.7
v52	979.2	1181.7	1193.0
v53	990.5	1190.3	1194.4
v54	993.0	1195.2	1205.5
v55	1000.4	1248.2	1247.1

v56	1003.7	1273.9	1265.9
v57	1004.8	1287.7	1270.0
v58	1007.5	1305.9	1310.5
v59	1018.1	1319.5	1317.1
v60	1019.1	1323.0	1324.9
v61	1026.1	1334.0	1348.1
v62	1030.7	1348.5	1361.2
v63	1044.0	1442.2	1364.3
v64	1060.0	1457.7	1465.2
v65	1060.7	1477.6	1470.2
v66	1078.6	1492.8	1477.0
v67	1080.5	1510.1	1494.1
v68	1093.8	1528.7	1527.3
v69	1103.9	1576.0	1535.0
v70	1121.6	1591.3	1578.3
v71	1141.0	1602.9	1603.1
v72	1167.9	1610.5	1619.2
v73	1181.2	1631.8	1636.4
v74	1184.0	1638.9	1645.4
v75	1184.5	3151.0	1650.6
v76	1189.8	3161.4	3168.1
v77	1190.3	3162.2	3169.0
v78	1208.2	3164.4	3170.0
v79	1243.1	3167.8	3182.3
v80	1266.6	3170.2	3183.2
v81	1280.2	3173.6	3185.8
v82	1292.6	3174.6	3197.8
v83	1307.7	3182.6	3200.3
v84	1317.5	3184.2	3203.4
v85	1323.1	3187.1	3215.7
v86	1327.0	3191.1	3217.2
v87	1331.1	3194.3	3223.0
v88	1361.4		
v89	1377.0		
v90	1459.8		
v91	1471.6		
v92	1480.3		
v93	1486.6		
v94	1499.4		

v95	1505.1
v96	1519.5
v97	1536.5
v98	1590.4
v99	1602.7
v100	1605.1
v101	1619.8
v102	1625.7
v103	1630.7
v104	1638.7
v105	1644.0
v106	3154.2
v107	3157.2
v108	3160.0
v109	3160.3
v110	3164.3
v111	3167.3
v112	3167.9
v113	3169.5
v114	3174.7
v115	3175.2
v116	3176.8
v117	3177.5
v118	3184.2
v119	3185.8
v120	3186.4
v121	3188.3
v122	3192.9
v123	3193.3

	tsi6	tsi6p5	tsi7	tsi7p6	tsp5i8 	tsp5i9 
v1	-294.5	-807.7	-311.0	-917.2	-1610.9	-1679.5
v2	11.9	43.4	12.9	50.1	15.4	16.6
v3	34.1	75.0	32.9	60.3	20.8	24.9
v4	53.9	85.3	55.8	91.1	28.3	34.2
v5	112.3	167.4	115.1	174.4	52.4	51.0
v6	123.8	188.5	129.6	185.1	72.4	68.1
v7	176.5	245.7	186.7	265.4	80.7	83.1
v8	197.2	286.7	204.2	271.7	125.7	123.7

v9	363.0	309.1	367.3	333.5	140.5	135.6
v10	369.0	407.3	384.1	383.7	166.7	168.0
v11	399.5	417.9	399.8	419.4	177.9	179.8
v12	440.1	422.3	441.4	430.1	200.5	208.6
v13	475.2	444.2	449.2	438.1	256.4	245.0
v14	498.3	486.7	490.3	487.1	299.0	299.9
v15	516.2	502.5	516.2	517.5	329.1	322.2
v16	519.5	526.4	523.5	526.0	405.8	405.5
v17	570.7	538.7	568.2	544.9	409.1	415.7
v18	613.9	576.0	614.6	565.3	433.3	425.6
v19	625.3	580.4	629.7	583.8	441.3	445.1
v20	640.0	635.7	635.2	635.1	447.7	465.7
v21	693.9	637.7	695.0	643.1	484.5	485.8
v22	729.1	666.0	730.6	672.3	508.2	509.5
v23	736.7	713.2	748.2	712.3	532.2	530.7
v24	767.9	721.7	770.1	718.3	574.5	573.5
v25	789.5	748.2	776.1	760.2	588.0	590.9
v26	801.4	784.4	807.7	777.0	620.6	619.4
v27	809.6	794.6	819.7	783.7	622.4	623.1
v28	836.5	807.7	838.4	791.0	631.6	633.3
v29	855.9	824.1	843.6	834.6	669.6	656.0
v30	887.8	845.0	895.2	860.3	680.9	667.2
v31	904.7	864.1	903.7	869.9	702.4	700.6
v32	914.6	890.9	906.0	881.8	716.8	719.3
v33	958.7	921.6	953.3	915.2	732.0	730.0
v34	970.2	944.6	966.8	943.0	738.5	739.8
v35	971.3	978.1	971.1	957.9	752.5	766.8
v36	984.7	982.7	988.6	971.9	774.4	783.4
v37	997.6	989.4	995.9	990.5	801.3	794.2
v38	998.7	992.9	999.6	991.6	810.0	806.9
v39	1003.9	1003.3	1003.7	999.7	824.0	843.0
v40	1024.9	1009.6	1018.5	1008.4	846.3	846.4
v41	1037.6	1021.8	1032.0	1020.6	849.0	861.2
v42	1050.2	1048.2	1045.0	1033.0	885.8	864.3
v43	1056.4	1055.2	1057.8	1044.9	890.8	911.4
v44	1081.3	1087.8	1081.9	1061.2	914.5	916.8
v45	1143.1	1105.3	1140.4	1106.4	936.4	933.9
v46	1165.4	1138.0	1163.3	1156.2	965.7	943.7
v47	1170.7	1169.9	1173.6	1175.3	977.7	972.9

v48	1178.5	1184.1	1178.6	1183.4	979.4	978.2
v49	1184.6	1186.3	1183.8	1185.0	984.3	985.1
v50	1185.2	1203.8	1185.4	1209.1	993.0	991.5
v51	1222.0	1207.5	1227.3	1218.4	994.1	994.1
v52	1265.0	1237.6	1271.3	1251.9	1001.0	1002.2
v53	1288.4	1270.1	1292.7	1288.4	1003.8	1008.6
v54	1319.9	1308.8	1321.0	1297.4	1004.6	1017.2
v55	1328.4	1309.9	1328.8	1316.0	1019.2	1021.6
v56	1372.0	1346.0	1381.3	1353.5	1044.4	1032.6
v57	1381.9	1362.0	1395.5	1374.7	1046.3	1051.7
v58	1419.5	1378.3	1421.3	1388.9	1054.2	1057.0
v59	1469.0	1423.7	1469.5	1409.9	1079.1	1066.4
v60	1479.8	1467.5	1479.3	1461.6	1083.1	1078.2
v61	1487.6	1482.8	1486.6	1486.9	1086.1	1091.8
v62	1492.5	1489.7	1490.2	1493.9	1123.0	1104.9
v63	1540.0	1530.3	1536.1	1532.4	1144.0	1140.8
v64	1581.1	1545.1	1580.9	1534.6	1172.0	1169.5
v65	1590.0	1594.5	1587.0	1590.3	1175.9	1177.9
v66	1608.1	1614.9	1626.2	1620.4	1181.2	1184.5
v67	1627.4	1619.5	1627.8	1634.5	1186.7	1189.5
v68	1654.4	1642.6	1645.4	1643.8	1188.4	1193.6
v69	3143.8	1655.2	3143.4	1653.6	1190.3	1204.0
v70	3153.3	3160.7	3153.1	3160.1	1211.0	1206.4
v71	3158.2	3162.6	3156.8	3162.6	1236.8	1215.7
v72	3161.0	3164.4	3159.1	3163.1	1241.8	1237.1
v73	3162.5	3169.9	3162.1	3165.6	1275.4	1296.3
v74	3163.8	3172.5	3162.4	3169.3	1287.8	1310.9
v75	3169.6	3177.6	3166.4	3173.5	1313.7	1317.6
v76	3170.2	3179.5	3169.0	3178.1	1325.6	1327.3
v77	3176.1	3185.4	3175.7	3179.8	1331.0	1352.3
v78	3178.0	3186.7	3178.1	3185.8	1365.7	1359.2
v79	3184.2	3190.7	3184.4	3190.5	1368.0	1364.8
v80	3188.9	3192.6	3188.6	3191.1	1387.7	1368.2
v81	3190.7	3201.8	3189.5	3193.3	1428.8	1414.0
v82					1461.0	1463.9
v83					1475.3	1477.7
v84					1482.5	1484.2
v85					1495.3	1485.1
v86					1504.0	1504.8

v87					1507.5	1528.0
v88					1548.6	1533.4
v89					1590.3	1597.8
v90					1605.0	1603.8
v91					1617.0	1617.1
v92					1626.7	1627.5
v93					1630.3	1635.4
v94					1637.6	1644.3
v95					1661.3	1650.6
v96					3154.6	3153.7
v97					3157.9	3157.5
v98					3159.3	3160.3
v99					3160.6	3160.4
v100					3162.4	3160.6
v101					3165.2	3166.8
v102					3170.0	3167.2
v103					3170.8	3170.1
v104					3174.9	3172.9
v105					3175.9	3176.2
v106					3176.6	3176.8
v107					3185.4	3181.9
v108					3186.5	3182.6
v109					3187.3	3186.0
v110					3190.1	3187.4
v111					3200.3	3191.6
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	tsp5i9 (H)	tsp5i8 (H)	tsi8i10	tsi9i11	tsi10p7	tsi11p7
v1	-959.1	-890.5	-444.5	-423.2	-870.9	-899.9
v2	37.3	42.6	84.7	80.5	104.3	106.1
v3	70.7	75.6	101.3	101.5	123.3	118.0
v4	82.9	81.7	160.2	169.9	170.7	167.4
v5	155.2	167.4	191.1	184.3	205.0	204.8
v6	167.9	177.6	254.8	231.3	252.2	252.5
v7	210.7	180.8	262.3	288.5	286.1	291.8
v8	242.0	241.1	352.0	352.4	347.5	353.3
v9	292.8	261.1	407.1	399.2	374.7	387.3
v10	316.0	298.7	420.7	425.9	436.6	431.9
v11	347.9	315.6	442.4	444.1	445.4	456.3
v12	416.6	408.7	478.1	474.5	461.0	466.0

v13	419.4	427.3	509.8	508.2	475.6	472.8
v14	457.8	444.4	520.4	533.6	487.6	492.4
v15	483.5	483.7	547.8	557.7	495.3	501.6
v16	503.9	507.3	568.3	582.0	570.9	571.6
v17	528.3	531.5	599.7	610.3	574.4	572.7
v18	572.6	569.4	616.7	612.4	577.3	576.7
v19	585.6	585.5	647.8	648.5	629.7	629.8
v20	624.8	620.7	688.4	683.4	633.2	638.0
v21	632.6	628.5	715.6	728.8	657.3	654.1
v22	660.7	667.8	751.9	750.2	687.4	682.0
v23	702.0	706.4	769.6	760.5	753.0	752.3
v24	719.7	726.4	775.3	788.4	762.6	759.6
v25	762.3	751.6	793.4	804.3	777.2	776.7
v26	781.7	768.8	804.7	814.9	790.3	795.9
v27	790.4	800.1	825.6	838.4	800.7	800.8
v28	805.8	809.6	864.0	859.3	819.0	819.7
v29	835.4	823.8	870.7	880.8	851.3	852.4
v30	836.8	844.7	879.8	898.1	890.9	884.6
v31	863.8	873.5	909.7	920.2	908.7	905.4
v32	898.6	890.8	948.8	952.8	914.0	920.9
v33	929.2	920.3	972.0	970.2	925.7	929.9
v34	934.9	936.0	977.0	978.8	958.8	956.5
v35	944.0	962.5	984.8	986.8	984.4	984.0
v36	964.4	973.3	990.8	989.1	990.7	990.8
v37	983.2	978.1	1004.9	1018.7	993.8	991.7
v38	991.1	984.4	1041.5	1035.7	994.1	993.8
v39	994.3	993.0	1055.3	1042.2	1045.7	1041.9
v40	1009.0	1000.0	1080.2	1068.9	1046.5	1042.1
v41	1021.4	1003.4	1117.7	1090.8	1068.7	1064.5
v42	1030.0	1018.1	1141.4	1138.1	1109.4	1109.4
v43	1053.5	1046.8	1156.4	1166.8	1124.4	1115.8
v44	1071.6	1055.6	1177.3	1177.5	1161.0	1164.7
v45	1098.9	1085.5	1181.6	1191.0	1184.8	1182.1
v46	1106.3	1129.7	1202.4	1201.8	1185.5	1187.5
v47	1134.2	1144.9	1227.0	1210.9	1209.1	1208.9
v48	1168.3	1172.0	1250.4	1243.6	1234.9	1237.6
v49	1184.5	1181.6	1266.6	1285.3	1254.0	1258.3
v50	1198.5	1188.1	1316.3	1318.9	1294.1	1294.5
v51	1207.1	1211.2	1323.6	1336.1	1322.1	1318.5

v52	1213.5	1237.1	1360.9	1361.0	1340.7	1333.6
v53	1240.7	1257.1	1373.2	1382.6	1386.4	1395.7
v54	1307.5	1277.5	1406.7	1419.0	1399.9	1398.2
v55	1311.5	1313.1	1441.5	1449.8	1428.0	1439.9
v56	1351.0	1323.1	1462.8	1458.1	1458.2	1455.8
v57	1360.5	1365.9	1474.8	1467.4	1468.4	1472.3
v58	1364.4	1387.2	1489.1	1506.7	1490.6	1481.5
v59	1397.1	1428.3	1523.9	1516.2	1505.7	1508.5
v60	1461.7	1447.8	1569.6	1566.2	1523.6	1526.3
v61	1471.6	1475.4	1585.5	1584.8	1609.0	1589.1
v62	1483.3	1486.4	1600.0	1600.2	1618.8	1626.9
v63	1519.6	1500.7	1620.2	1628.6	1633.8	1639.3
v64	1532.9	1548.8	1635.1	1648.7	1645.5	1640.0
v65	1594.1	1579.5	3129.6	3130.4	1648.6	1658.3
v66	1617.1	1616.1	3153.5	3153.7	3163.2	3162.8
v67	1634.9	1629.5	3159.4	3160.1	3163.7	3163.4
v68	1644.5	1637.0	3161.4	3163.0	3164.6	3165.0
v69	1651.5	1661.4	3162.7	3166.3	3170.1	3171.6
v70	2267.1	2335.5	3169.5	3169.0	3174.3	3173.5
v71	3159.5	3159.7	3173.9	3172.4	3177.1	3174.5
v72	3161.8	3160.2	3175.6	3177.9	3180.0	3182.4
v73	3162.3	3163.2	3185.1	3181.1	3186.7	3186.1
v74	3168.6	3166.7	3186.0	3185.7	3188.2	3186.9
v75	3168.7	3171.5	3187.5	3191.6	3191.4	3192.8
v76	3175.0	3176.0				
v77	3177.8	3176.5				
v78	3183.3	3186.4				
v79	3184.2	3188.3				
v80	3189.0	3189.8				
v81	3192.2	3201.7				

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